Abstract

Many problems in mechanical engineering and physics are reduced to studying the following question. There is a variational problem to minimize a sum of quadratic and linear functionals. The linear functional is stochastic, therefore the minimum value is random. How to find the probability density function of the minimum value? Such type of problem appears in statistical mechanics of fluid motion, Kosterlitz-Thouless phase transition, brittle-to-ductile transition in solids, reaction of cracked bodies to random excitation, lubrication theory, etc. It is shown in this paper that the probability density function of minimum values is determined by some variational problem. The features of this variational problem are discussed.

1 Introduction

The problem under consideration is closely related to the homogenization problem and can be formulated as follows. Consider a quadratic functional

$$I(u) = \frac{1}{2} (Au, u) - (l, u).$$

Here $(Au, u)$ and $(l, u)$ stand for quadratic and linear parts of the functional $I(u)$. A typical example is the case of a scalar function $u$ defined in some bounded region $V$ of $n$-dimensional space, and

$$[Au, u] = \int_V \frac{\partial u}{\partial x^i} \frac{\partial u}{\partial x^j} d^nx, \quad (l, u) = \int_V \rho(x) u(x) d^n x.$$  

If $u = 0$ at $\partial V$ then $A$ can be viewed as a positive operator, $A = -\Delta$ ($\Delta$ is the Laplace operator).

Quadratic functional $(Au, u)$ is assumed to be positive.

If $u$ is a vector of $m$-dimensional space $R^m$, then $A$ is a positive symmetric matrix, $l$ is a vector in $R^m$, and $(\cdot, \cdot)$ is the usual scalar product.

Denote the minimizing element of $I(u)$ by $\bar{u}$. The minimum value of the functional $I(u)$ is equal to $-\frac{1}{2} \left( A \bar{u}, \bar{u} \right)$ and always negative. In physical problems, the quadratic part of $I(u)$ has usually the sense of energy while the linear functional represents the external action on the system. In what follows the negative minimum value of $I(u)$ is called energy.
Let the linear functional be stochastic. In the case of the functional (1.2) that means that $\rho(x)$ is a stochastic field. In the problems considered here the randomness comes into play through the dependence of the linear functional on a large number of independent random variables, $r_1,...,r_N$. The total set $(r_1,...,r_N)$ is denoted by $r$. So, $I = I(u, r)$, and the negative minimum value of $I$, energy, is a function of $r$, i.e. it is a random variable. The problem is to find the probability density function of energy.

Here we solve this problem for two cases: in the case when the linear functional is a sum of $N$ small (in the order of $1/N$) linear statistically independent functionals,

$$
(l, u) = \frac{1}{N} \sum_{i=1}^{N} (l_i(r_i), u) \tag{1.3}
$$

and when each term is much larger, in the order of $1/\sqrt{N},$

$$
(l, u) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} (l_i(r_i), u). \tag{1.4}
$$

In the latter case we assume that the average value of each term of the sum is zero.

Each member of the sum depends only on one random variable. The $i$th random variable has the probability density function, $f_0$. Large external actions (1.4) will be discussed in section 13, while here we formulate the results for small excitations (1.3). In this case, the probability density function of energy is

$$
f(E) = \text{const} \times e^{N \hat{S}(E)} \tag{1.5}
$$

where $\hat{S}$ is the maximum non zero stationary value of the functional

$$
S(E, z, u) = Ez + \frac{z}{2} (Au, u) + \frac{1}{N} \sum_{i=1}^{N} \ln \int e^{-z[l_i(r), u]} f_0^i(r) dr. \tag{1.6}
$$

The stationary points of the functional (1.6) are sought with respect to real variable $z$ and function $u$. The constant in (1.5) can be found from the normalizing condition,

$$
\int f(E) dE = 1.
$$
If all linear functionals in (1.3) are the same

\[ (l, u) = \frac{1}{N} \sum_{i=1}^{N} (l_0(r_i), u), \]

and the random variables have the same probability distribution, \( f_0(r) \), then the functional \( S(E, z, u) \) takes especially simple form

\[ S(E, z, u) = Ez + \frac{z}{2}(Au, u) + \ln \int e^{-z(l_0(r),u)} f_0(r) \, dr. \]

(1.8)

We will discuss mostly this case; an extension to a more general case (1.3) is straightforward.

It is often convenient to make a change of the variable,

\[ u \rightarrow v = zu, \]

to eliminate the dependence of the last term in (1.8) on \( z \) and to make obvious the convexity of \( S \) with respect to \( z \):

\[ S(E, z, v) = Ez + \frac{1}{2z}(Av, v) + \ln \int e^{-(l_0(r),v)} f_0(r) \, dr. \]

(1.9)

The stationary points of the functional (1.9) are denoted by \( \beta, \gamma \). We do not use the symmetric notation \( \gamma \) for the stationary point with respect to \( z \) because, in physical problems, \( \gamma \) has usually the sense of the inverse temperature \( \beta \). Obviously,

\[ \frac{d\gamma}{dE} = \beta, \]

therefore the function \( \gamma (E) = S(E, \beta, \gamma) \) has the sense of entropy. We call the functional \( S(E, z, v) \) the entropy functional.

Formula (1.5) solves, in fact, a problem of large deviations. Indeed, the sum (1.7) converges to the averaged linear functional

\[ (\bar{l}, u) = \int (l_0(r), u) f_0(r) \, dr \]

(1.10)

and the most probable value of energy \( E \) corresponds to the minimum value of the averaged functional,

\[ -E = \min_u \left[ \frac{1}{2} (Au, u) - (\bar{l}, u) \right]. \]

(1.11)
Function $\hat{S}(E)$ should have the maximum value at $E = \bar{E}$. If $E - \bar{E}$ is small, in the order of $1/\sqrt{N}$, formula (1.5) yields the central limit theorem. Finite $E - \bar{E}$ corresponds to large deviations of energy from the most probable value.

We call the functionals under consideration weakly stochastic because randomness enters in the linear part. Homogenization problems correspond to strong stochasticity: the randomness of the quadratic part. As will be seen from the derivation the results formulated admit a generalization to the strongly stochastic functionals in some cases.

It is easy to explain why the entropy functional appears in the formula (1.5).

As in any probabilistic problem with independent random variables, it is worth considering the Fourier transform of the probability density

$$Me^{Nz \min_u I(u)}$$

(1.12)

where $M$ is the mathematical expectation, and $z$ is a point on the imaginary axis. It is desirable to find a way to “change the order” of averaging with respect to probabilistic measure and minimization in (1.12). If we can do that, then the original problem is reduced to some other variational problem. A key to performing such a change is the following observation:

Let $u$ and $l$ be vectors in $m$-dimensional space. In this case $A$ is a positive $m \times m$ matrix, and $(\cdot, \cdot)$ is the usual scalar product. It is well known that the integral of the exponent of a quadratic form has the value:

$$\int e^{-\frac{1}{2}(Au,u) + (l,u)} d^m u = e^{\frac{1}{2}(A^{-1}l,l)} \sqrt{\frac{(2\pi)^m}{\det A}},$$

(1.13)

where $A^{-1}$ is the inverse matrix. The remarkable point is that this relation can be written in the from

$$e^{-\min_u \left[ \frac{1}{2}(Au,u) - (l,u) \right]} = \int e^{-\frac{1}{2}(Au,u) + (l,u)} d^m u.$$

(1.14)

We presented $\exp \left[ - \min_u I(u) \right]$ as an integral. Now the order of integration and averaging with respect to probabilistic measure can be changed. Doing this in the Fourier representation of the probability density function,

$$f(E) = \frac{N}{2\pi i} \int_{-i\infty}^{+i\infty} Me^{NEx + Nz \min_u I(u)} dz$$

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we obtain

$$f(E) = \text{const} \times \int \int e^{NS_m(E, z, u)} d^m v d z,$$

(1.15)

where $S_m$ is an $m$-dimensional truncation of the entropy functional. We have then to find the asymptotics of the integral (1.15), if $N, m \to \infty$. Formula (1.6) corresponds to the case when the asymptotics of the integral (1.15) is determined by the maximum stationary value of $S_m$ as in the steepest descent method. Unfortunately, the steepest descent method cannot be applied directly because it assumes that $m \ll N$, while we are interested in the case $m \gg N$. Thus, we go another way: we establish the identity,

$$f(E) = R(N, E) e^{N \tilde{S}(E)},$$

(1.16)

where the prefactor $R$ is determined by some explicit formulas.

It turns out that in many problems $R(N, E)$ does not depend on $E$ in the limit $N \to \infty$, and the formula (1.5) holds.

Weakly stochastic variational problems are of great interest in various problems of physics and mechanics some of which are discussed below. The plan of the paper is as follows. We begin with a simple example supporting formulas (1.5), (1.9) (section 2). In the next five sections some physical problems are considered solutions of which are reduced to a weakly stochastic variational problem. In each problem the entropy functional $S(E, z, u)$ is written down. Some features of the variational problem for the entropy functional and the meaning of its solutions are discussed in section 8. Justification of (1.5) based on the identity (1.16) is derived in section 9. In this section the various forms of the prefactor $R$ are established. Another derivation of (1.16) is given in section 10. In section 11, under some assumptions, the prefactor is shown to be independent on $E$ in the limit $N \to \infty$, and, thus, formula (1.5) holds. The necessity of one of the assumptions is supported by a counterexample in section 12. The last section concerns with the case of large excitations. Appendices contain the derivation of the basic identity (1.16) for the functional (1.3), an outline of the proof of the formula for conditional probability (8.8) and discussion of negative temperature states for a one-dimensional problem which admits a complete investigation.
2 An example

We begin with the simplest possible case, a quadratic function $I(u)$ of one
real variable,

$$l = \frac{1}{N} \sum_{i=1}^{N} l_{0}(r_{i})$$

where $r_{i}$ are independent random variables. Without loss of generality we
may change variables and put $l_{0}(r) \equiv r$. Then, in accordance with (1.9),

$$S(E, z, v) = E z + \frac{1}{2} v^{2} + \ln \int e^{-rv} f_{0}(r) dr. \quad (2.17)$$

The stationary points with the respect to $z$ are determined by the equation

$$\frac{v^{2}}{2\beta^{2}} = E \quad \text{or} \quad \beta = \pm \sqrt{\frac{v^{2}}{2E}}.$$

At these stationary points,

$$S(E, v) = \pm \sqrt{2E} |v| + \ln \int e^{-rv} f_{0}(r) dr. \quad (2.18)$$

To determine $\hat{S}(E)$ one has to find the stationary points $\hat{v}$ of the function
(2.18) at which $S(E, v)$ has the largest value.

Let us compare this statement with the exact formula for the probability
density of min $I(u)$, which can be found by the steepest
descent method. Indeed, since min $I(u) = -1/2l^{2}$,

$$f(E) = \left[ g\left(\sqrt{2E}\right) + g\left(-\sqrt{2E}\right) \right] \frac{1}{\sqrt{2E}}, \quad (2.19)$$

where $g(\xi)$ is the probability density function of the random variable $l$. For
$g(\xi)$ we have

$$g(\xi) = M \delta \left( \xi - \frac{1}{N} \sum l_{i} \right) = \frac{1}{2\pi i} M \int_{-i\infty}^{i\infty} e^{z(\xi - \frac{1}{N} \sum l_{i})} dz =$$

$$= \frac{N}{2\pi i} \int_{-i\infty}^{i\infty} e^{Nz\xi} \left( \int e^{-zr} f_{0}(r) dr \right) dz =$$
\[ g(\xi) = \frac{N}{\sqrt{2\pi}} S''(\xi) e^{NS_1(\xi)}. \] (2.22)

Plugging (2.22) into (2.19) we see that one of the terms, \( \exp \left( NS_1 \left( -\sqrt{2E} \right) \right) \), which correspond to the smaller value of \( S_1 \), is negligible compared with the other one. The prefactor \( (\sqrt{2E} S''(\sqrt{2E}))^{-1} \) is not essential since it corresponds to small correction to \( S_1 \). Thus one has to consider the stationary points of function \( S_1(v, \sqrt{2E}) \) and \( S_1(v, -\sqrt{2E}) \) with respect to \( v \) and find the stationary point at which the stationary value is the largest. The graphs of two functions \( S_1(v, \sqrt{2E}) \) and \( S_1(v, -\sqrt{2E}) \) coincide with the graphs of two branches of the function (2.18). Therefore, the stationary points and the stationary values coincide as well. The only point, \( v = 0 \), needs special attention since the function (2.18) is not smooth at this point. The point \( v = 0 \) is the limit of stationary points if \( \sqrt{2E} \to < r > \). If \( \sqrt{2E} \neq < r >, v = 0 \) is not a stationary point of smooth function (2.17), thus the variational problem (2.17) yields the same result as the exact formula. Coincidence in the case \( \sqrt{2E} = < r > \) we obtain from continuity tending \( \sqrt{2E} \) to \( < r > \).

3 Statistical mechanics of point vortices

Statistical mechanics of point vortices studies the probabilistic and thermodynamic properties of the Hamiltonian system with the Hamilton function

\[ H = \frac{1}{2} \sum_{i \neq j} \gamma_i \gamma_j G(r_i, r_j) \] (3.23)
where \( r_1 \ldots r_N \) are points of two – dimensional bounded region \( V \), \( G(r, r') \) is Green’s function of the Laplace operator with zero boundary conditions in this region. The \( x \)-components of two-dimensional vectors \( r_i \) are the generalized coordinates of the system while the \( y \)-components are the corresponding generalized momenta. It is assumed that the system of point vortices moves ergodically (note that all low-dimensional numerical experiments does not support this hypothesis; it might be, however, that ergodicity takes place approximately for large \( N \)). Statistical mechanics of point vortices has a long and rich history; a list of references on the subject is given in [3]. All statistical and thermodynamic properties of the ergodic system of vortices can be expressed in terms of probability density function of energy (3.23) if \( r_1 \ldots r_N \) are placed randomly and independently in region \( V \) [2, 3].

The kinetic energy is the negative minimum value of the functional

\[
-H(r_1 \ldots r_N) = \min_u I(u, r)
\]

\[
I(u) = \frac{1}{2} (Au, u) - (l, u), \quad (Au, u) = \int_V \frac{\partial u}{\partial x^\alpha} \frac{\partial u}{\partial x^\alpha} d^2x, \quad (l, u) = \int_V \omega u d^2x
\]

(3.24)

\[
\omega = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \delta(x - r_i), \quad \gamma_i = \frac{\sigma_i}{N}.
\]

(3.25)

Minimum is sought on the set of all functions \( u \) taking zero values at the boundary \( \partial V \) of the region \( V \). Function \( u \) is the stream function of the flow, \( \omega \) is vorticity.

\( \delta \)-functions in (3.25) yield infinite energy, and the functional \( I(u) \) needs a regularization. One way is to remove self–interaction energy and conduct summation in (3.23) over \( i \neq j \). Another way is to change \( \delta(x) \) by a finite function, \( \delta_\varepsilon(x) \), which is equal to \( 1/\varepsilon \) in a small circle of area \( \varepsilon \) centered at the point \( x \) and equal to zero outside of this circle. Consider the second way.

The variational problem for the functional (3.24) is a weakly stochastic variational problem. Thus, probability density function of energy is given by formula (1.5) where \( S(E) \) is the maximum stationary value of the functional

\[
S_\varepsilon(E, z, \gamma) = Ez + \frac{1}{2z} \int_V \frac{\partial u}{\partial x^\alpha} \frac{\partial u}{\partial x^\alpha} d^2x + \frac{1}{N} \sum_{i} \ln \frac{1}{|V|} \int_V e^{-\gamma_i \sigma_i(x)} d^2r
\]

(3.26)
where \( v_\varepsilon(x) \) is the function \( v(x) \) averaged over the circle vicinity of radius \( \varepsilon \) centered at the point \( x \). The sum in (3.26) is, in fact, independent on \( N \) if there are a few values of \( \sigma_i \), say, \( \sigma_1, \ldots, \sigma_k \), which appear with frequencies \( c_1, \ldots, c_k \). In this case,

\[
S_\varepsilon(E, z, v) = Ez + \frac{1}{2\varepsilon} \int_{\mathbb{V}} \frac{\partial v}{\partial x^\alpha} \frac{\partial v}{\partial x^\beta} d^2 x + \sum_a c_a \ln \frac{1}{|\mathbb{V}|} \int_{\mathbb{V}} e^{-\sigma_a v_\varepsilon(x)} d^2 x.
\]

(3.27)

The stationary values of the functional \( S_\varepsilon \) converges for \( \varepsilon \to 0 \) to the stationary values of the functional

\[
S(E, z, v) = Ez + \frac{1}{2z} \int_{\mathbb{V}} \frac{\partial v}{\partial x^\alpha} \frac{\partial v}{\partial x^\beta} d^2 x + \sum_a c_a \ln \frac{1}{|\mathbb{V}|} \int_{\mathbb{V}} e^{-\sigma_a v(x)} d^2 x.
\]

(3.28)

The functional (3.28) was obtained from other reasoning in [2].

4 The Kosterlitz-Thouless phase transition

Consider now another problem which is reduced to studying a weakly stochastic functional, so-called Kosterlitz-Thouless phase transition. Originally, this problem was posed by Kosterlitz and Thouless for dislocations in solids [15], but later on it was found to be quite common in various fields. Herein, we discuss this problem for the case of dislocations in linearly elastic solids, but we begin with a more general problem of the internal stresses in solids caused by residual strains.

Let \( V \) be a bounded three-dimensional region and \( w_i \) are the components of the displacement vector defined in \( V \). The components of the total strain tensor are

\[
\varepsilon_{ij} = \frac{1}{2} \left( \frac{\partial w_j}{\partial x_i} + \frac{\partial w_i}{\partial x_j} \right).
\]

(4.29)

Let each material element \( x \) have the residual strains \( \varepsilon_{ij}^0(x) \). By definition, elastic strains are \( \varepsilon_{ij} - \varepsilon_{ij}^0(x) \). The true displacement field minimizes the functional

\[
I(w) = \int_V U d^3 x - \int_{\partial V} f^i w_i d^2 x,
\]
\[ U = \frac{1}{2} A^{ijkl} (\varepsilon_{ij} - \varepsilon_{ij}(x)) (\varepsilon_{ij} - \varepsilon_{ij}(x)), \]

where \( A^{ijkl} \) are the elastic moduli.

There is a scalar version of this problem, so-called anti-plane deformation, when only one component of the displacement vector \( w_3 \equiv w \) is not zero and depends on \( x_1, x_2 \) only while the nonzero components of the residual strains are \( \varepsilon^0_\alpha \equiv \varepsilon^0_\alpha (x_1, x_2) \) (Greek indices run values 1,2). Then

\[
I(w) = \int_V \frac{1}{2} A^{\alpha\beta} \left( \frac{\partial w}{\partial x_\alpha} - \varepsilon^0_\alpha \right) \left( \frac{\partial w}{\partial x_\beta} - \varepsilon^0_\beta \right) d^2 x - \int f w ds. \quad (4.30)
\]

For simplicity we focus on this scalar version of the general problem assuming in addition that the elastic body is isotropic: \( A^{\alpha\beta} = \mu \delta^{\alpha\beta} \).

If the residual strains are potential,

\[ \varepsilon^0_\alpha = \frac{\partial^0 w}{\partial x^\alpha}, \]

then, for zero external traction \( f \), no internal stresses develop: it is clear that the minimum value of the functional (4.30), elastic energy, is zero, and minimum is achieved for \( w = 0 \). Nontrivial stress field appears only if the strains \( \varepsilon^0_\alpha \) are “incompatible”, i.e.

\[ \frac{\partial \varepsilon^0_1}{\partial x^2} \neq \frac{\partial \varepsilon^0_2}{\partial x^1}. \]

Incompatibility is measured by the so-called dislocation density,

\[ \rho = \frac{\partial \varepsilon^0_1}{\partial x^2} - \frac{\partial \varepsilon^0_2}{\partial x^1}. \quad (4.31) \]

Similar measure appears in the 3D case.

If the residual strains are random we have a problem of the type considered above. Various physical problems yield different types of randomness.

Dislocation is a defect in crystal lattice. Internal stresses caused by dislocations can be found by modeling this crystal lattices by an elastic body with residual strains. The residual strains \( \varepsilon^0_\alpha \) are not equal to zero in a thin
strip the thickness of which is equal to the interatomic distance. The residual strains \( \varepsilon^0_\alpha \) are constant along the strip except the edges where \( \varepsilon^0_\alpha \) change smoothly to zero to eliminate the singularities in the stress field. Obviously, the dislocation density \( \rho \) is not equal to zero only in these areas which are called the dislocation cores.

The dual variational problem for the functional (4.30) has the same form as the point vortex problem of section 3. Indeed, following the general recipe for construction of the dual variational problem (see, for example, [1]) we have

\[
I = \min_w I(w) = \\
= \max_{\sigma^\alpha} \left[ \int_V \left[ \sigma^\alpha \left( \frac{\partial w}{\partial x^\alpha} - \varepsilon^0_\alpha \right) - \frac{1}{2\mu} \sigma^\alpha \sigma^\alpha \right] d^2x - \int_{\partial V} f(s) w \, ds \right] = \\
= \max_{\sigma^\alpha} \left[ - \int_V \left( \frac{1}{2\mu} \sigma^\alpha \sigma^\alpha + \sigma^\alpha \varepsilon^0_\alpha \right) d^2x \right].
\]  

(4.32)

In the last variational problem the maximum is sought on the set of all stress field \( \sigma^\alpha(x) \) such that

\[
\frac{\partial \sigma^\alpha}{\partial x^\alpha} = 0, \quad \sigma^\alpha \nu_\alpha = f(s) \quad \text{at} \quad \partial V. 
\]  

(4.33)

The general solution of (4.33) has the form

\[
\sigma^\alpha = e^{\alpha\beta} \frac{\partial u}{\partial x^\beta}, \quad u|_{\partial V} = u^0(s),
\]  

(4.34)

where \( e^{\alpha\beta} \) are the Levi-Civita symbols, \( u \) is the stress function, and the boundary values of \( u \) is found from the relation

\[
\frac{d}{ds} u^0 = f(s).
\]

Plugging (4.34) in (4.32) we obtain

\[
I = -\min_u \int_V \left[ \frac{1}{2\mu} \frac{\partial u}{\partial x^\alpha} \frac{\partial u}{\partial x^\alpha} + e^{\alpha\beta} \frac{\partial u}{\partial x^\beta} \varepsilon^0_\alpha \right] d^2x =
\]
\[ \begin{aligned}
&= -\min_u \int_V \left[ \frac{1}{2\mu} \frac{\partial u}{\partial x^\alpha} \frac{\partial u}{\partial x^\beta} - \rho u \right] \, d^2x - \int \frac{e^{\beta \nu \alpha \beta \varepsilon_\alpha^0 \varepsilon_\beta^0}}{\partial V} u \, ds. \\
\text{(4.35)}
\end{aligned} \]

Here minimum is taken on the set of all functions \( u \) having the prescribed values \( \hat{u} \) at the boundary. Comparing this problem with the problem of determining the velocity field by known vorticity \( \omega \), we see that the stress function \( u \) corresponds to the stream function of the vortex flow while the dislocation density \( \rho \) corresponds to vorticity \( \omega \). Dislocations are analogous to vortex blobs, and for a single dislocation centered at the point \( r \)

\[ \rho = b \delta_r(x - r). \]

Dislocations in the antiplane problem may have two signs which are determined by the sign of the constant \( b \).

Consider the dislocations positioned at the points \( r_1, ..., r_N \). Then \( L \) is a function of \( r_1, ..., r_N \):

\[ L = L(r_1, ..., r_N). \]

Under some assumptions of physical nature, the probability to find dislocations at these positions is

\[ f(r_1, ..., r_N) = \frac{1}{Z} e^{-\beta \bar{L}(r_1, ..., r_N)} \]

where \( \beta \) is the inverse temperature \( (\beta = 1/T, \ T \text{ is the absolute temperature}). \)

The normalizing factor \( Z \) is a function of \( \beta \)

\[ Z(\beta) = \int e^{-\beta \bar{L}(r_1, ..., r_N)} \, dr_1...dr_N. \]

Some conclusion on dislocation behavior can be drawn from the calculation of energy of a single dislocations and a pair of dislocations. That can be done explicitly. Energy of two closely positioned dislocations of the same sign is much greater than the energy of two dislocations of the opposite signs. Energy of a single dislocation is also much greater than energy of two close dislocations of the opposite signs (dipole pair). Therefore, typically, if dislocations appear due to thermal fluctuations they appear as dipoles. This changes at high temperature: probability of a pair of dislocations to dissolve, i.e. to be far away, becomes considerable. The explicit estimation gives unrealistically high values of temperature for which
dissolving occurs. Kosterlitz and Thouless [15] suggested that the dislocation pairs may dissolve actually for much smaller temperature due to interaction(screening) which decreases $L$. Function $Z(\beta)$ may serve as an integral characteristic of dissolving. At the critical inverse temperature of dissolving, $\beta_c$, $Z(\beta)$ should have some steep change.

Calculation of the interaction energy and $\beta_c$ is a nonelementary task. Kosterlitz and Thouless offered a recipe to determine approximately the interaction energy and the critical temperature. The recipe seems quite questionable for me. It is very interesting to compare it with the exact relations following from the approach outlined. Indeed, the function $Z(\beta)$ can be found from (4.36)

$$Z(\beta) = |V|^N \int e^{\beta E} f(E) dE. \quad (4.37)$$

where $f(E)$ is the probability density function of (negative) minimum values of the functional (4.35). The probability density function

is sought under condition that all dislocations are distributed homogeneously and independently over $V$. The probability density function is given by formula (1.5) where $S$ is the functional

$$S(E, z, v) = E z + \frac{1}{2z\mu} \int \frac{\partial v}{\partial x^a} \frac{\partial v}{\partial x^a} d^2 x + \frac{1}{N} \sum_i \ln \frac{1}{|V|} \int e^{-b_i v(r)} dr. \quad (4.38)$$

Comparison of $Z(\beta)$ determined by (4.37) and (4.38)
and Kosterlitz-Thouless approach is an interesting open problem.

5 Brittle-to-ductile transition

Any material fractures in a brittle way if its temperature is low enough. This means that cracks propagate without deformation of the surrounding material. Any material fractures in a ductile way if its temperature is high enough. This means that considerable material deformation develops in the vicinity of the crack tip, impeding further propagation of the crack. The remarkable phenomenon is that for many materials the transition from brittle to ductile behavior occurs in a very narrow temperature range, on the order of 3 to 5 °C. There is no clear understanding of the mechanism of brittle-to-ductile transition, although some proposals have been made in the pioneering
work by J. Rice and R. Thompson [20] and subsequent papers on dislocation generation based models [21, 19, 22, 7, 23, 25, 26]

and dislocation mobility – based models [4, 7, 6, 8, 10].

This is one the major challenges in the materials sciences, from both theoretical and practical points of view.

Recently, Khanta, Pope and Vitek [13, 14] put forth an idea that brittle-to-ductile transition is, in fact, a Kosterlitz-Thouless type transition. This means that the simultaneous appearance of a cloud of dislocations in the vicinity of the crack tip is much more probable than the successive appearance of the same dislocations. In other words, the creation of a cloud of dislocations is a collective phenomenon: dislocations help each other to appear.

To evaluate this idea one has to study the variational problem (4.35) complicated by the presence of a crack, a cut in the region \( V \) the sides of which are free surfaces. Similarly, a cut appears in the variational problem for the entropy functional \( S \) (4.38). This is another interesting open problem.

6 Elastic body under action of random external forces

Formulas (1.5), (1.6) determine the probability density function of energy of elastic bodies subjected to action of random external forces. Consider, for example, an elastic beam with the clamped edges bent by random forces applied at the points \( r_1, ..., r_N \). The true displacement gives the minimum value to the functional

\[
I(u) = \frac{1}{2} \int_0^l D \left( \frac{d^2u}{dx^2} \right)^2 \, dx - \sum_{i=1}^N \gamma_i u(r_i)
\]

(6.39)

where \( D \) is the bending rigidity and \( \gamma_i \) are the intensities of the external forces. Minimum is sought on the set of functions \( u(x) \) obeying the constraints

\[
\frac{du}{dx} = 0 \quad \text{at} \quad x = 0, l.
\]

(6.40)

Assuming that all forces are small, in the order of \( 1/N \),

\[
\gamma_i = \frac{\sigma_i}{N},
\]

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and points of application, \( r_i \), are independently distributed over the beam with the probability density \( f_0(r) \), we have for the entropy functional

\[
S(E, z, v) = Ez + \frac{1}{2z} \int_0^l D \left( \frac{d^2v}{dx^2} \right)^2 dx + \frac{1}{N} \sum_i \ln \int e^{-\sigma_i v(r)} f_0(r) dr. \quad (6.41)
\]

An interesting problem appears if an elastic body contains a crack. The functional \( I(u) \) has the form

\[
I(w) = \frac{1}{2} \int_V A^{ijkl} \varepsilon_{ij} \varepsilon_{kl} d^3x - \int_{\partial V} f_i w_i d^2x + \gamma |\Sigma|,
\]

where \( \varepsilon_{ij} \) are given by (4.29), \( |\Sigma| \) is the area of the crack and \( \gamma \) is the surface energy. Let

\[
f^i = \frac{1}{N} \sum_{\alpha=1}^{N} \varphi^i(x - r_\alpha)
\]

and \( r_1, ..., r_N \) are statistically independent and have the probability density \( f_0(r) \). Then

\[
S(E, z, v) = Ez + \frac{1}{2z} \int_V A^{ijkl} \frac{\partial v_j}{\partial x^l} \frac{\partial v_k}{\partial x^l} d^3x +
\]

\[
+ \gamma |\Sigma| + \ln \int e^{-\int_{\partial V} \varphi^i(x-r) v_i(x) dx} f_0(r) dr.
\]

The minimum is sought over all displacement field \( w \) and all possible extension of the crack. If the extension of crack increases \( I \) then the crack does not grow. One may expect that small forces can not cause the crack growth. However, some combinations of small forces may make the crack to develop. To find the probability of the crack growth one has to find the stationary points of the functional \( S \).

\section{7 Homogenization problems}

Consider a microinhomogeneous media, for example, a heat conducting body with a periodic microstructure. Let at each cell a source of heat is placed. The positions of heat sources are random and independent at each cell. Then
one may expect that formula (1.5) holds where \( \overset{\mathcal{S}}{S} \) is the maximum stationary value of the functional

\[
\begin{align*}
S(E, z, v) &= \quad \\
&= Ez + \frac{1}{2z} \int_v a(x) \frac{\partial v}{\partial x^k} \frac{\partial v}{\partial x^k} d^3x + \\
&\quad + \frac{1}{N} \sum_i \ln \int e^{-\varphi(x-r)\psi(x)} \psi(x) f_0(r) dr.
\end{align*}
\]

where \( a(x) \) is a periodic function of \( x \) and \( \varphi(x) \) is the source intensity. The functional (7.42) can be studied using the variational asymptotic method [1]. This yields the “homogenized” functional \( \mathcal{S} \)

\[
\mathcal{S}(E, z, v) = \quad \\
= Ez + \frac{1}{2z} \int_v \bar{a}(x) \frac{\partial \bar{v}}{\partial x^k} \frac{\partial \bar{v}}{\partial x^k} d^3x + \int_v \left[ \ln \int e^{-\varphi(x-r)\psi(x)} f_0(r) dr \right] d^3x.
\]

For general homogenization problem formula (1.5) should be valid, but the expression for entropy functional is different. One may try to use the identity (1.14) to determine the entropy functional. The difficulty is in randomness of \( \det A \). For the cases when \( \det A \) is not random or probabilistic properties of \( \det A \) are known, the entropy functional can be found from (1.14).

8 Some features of stationary points of entropy functional

Entropy functional (1.9) is convex with respect to \( v \) for positive \( z \) and nonconvex for negative \( z \). Therefore, there is the only stationary point for positive \( z \), and there might be many for negative \( z \). For negative \( z \), the variational problem for the entropy functional is a nonlinear eigenvalue problem.

Let us show that entropy \( \overset{\mathcal{S}}{S}(E) \) is negative at each stationary point,

\[
\overset{\mathcal{S}}{S}(E) \leq 0
\]
Each stationary point $\beta, \bar{\psi}$ of the entropy functional obeys the equations

$$
\frac{1}{2\beta^2}(A \bar{\psi}, \bar{\psi}) = E; \quad (8.44)
$$

$$
\frac{1}{\beta} A \bar{\psi} = \int l_0(r) e^{-l_0(r), \bar{\psi}} f_0(r) dr / \int e^{-l_0(r), \bar{\psi}} f_0(r) dr. \quad (8.45)
$$

Therefore, at a stationary point,

$$
\frac{1}{\beta}(A \bar{\psi}, \bar{\psi}) = \int (l_0(r), \bar{\psi}) e^{-l_0(r), \bar{\psi}} f_0(r) dr / \int e^{-l_0(r), \bar{\psi}} f_0(r) dr = 2\beta E. \quad (8.46)
$$

Denote the function of $r$, $(l_0(r), \bar{\psi})$, by $\psi(r)$, and by $J(\psi)$ the functional of $\psi$

$$
J(\psi) = \ln \int e^{-\psi(r)} f_0(r) dr
$$

Then

$$
\bar{S}(E) = J(\psi) + \int \psi(r) e^{-\psi(r)} f_0(r) dr / \int e^{-\psi(r)} f_0(r) dr =
$$

$$
= J(\psi) - \int \psi \frac{\delta J}{\delta \psi} dr \quad (8.47)
$$

where $\delta J/\delta \psi$ is the variational derivative of $J$.

For any convex functional $J(\psi)$ the following inequality is true

$$
J(\psi_1) - J(\psi_2) \geq \left( \frac{\delta J}{\delta \psi} \right)_{\psi=\psi_2} (\psi_1 - \psi_2) \quad (8.48)
$$

see, for example, [24]. Putting in (8.48) $\psi_1 = 0$, $\psi_2 = \psi$, and taking into account that $J(0) = 0$, we see that the expression (8.47) is always negative as claimed.

If a solution of equations (8.44), (8.45) exists for some positive $\beta$, it provides the maximum value of entropy. Indeed, let $\beta_1, \bar{\psi}_1$ and $\beta_2$, $\bar{\psi}_2$ be
two solutions of equations (8.44), (8.45). Denote by \( \hat{S}_1(E) \) and \( \hat{S}_2(E) \) the corresponding values of entropy. Then the inequality holds

\[
\hat{S}_1(E) - \hat{S}_2(E) \geq 2E(\beta_1 - |\beta_1|).
\] (8.49)

If \( \beta_1 > 0 \), then the right hand side of (8.49) is zero, and

we obtain the statement made. To derive (8.49) we note that

\[
\frac{1}{\beta_1} A \frac{\delta J}{\delta \hat{v}_1} = -\frac{\delta J}{\delta \hat{v}_1}, \quad \frac{1}{2\beta_1^2} (A \hat{v}_1, \hat{v}_1) = E;
\]

\[
\frac{1}{\beta_2} A \frac{\delta J}{\delta \hat{v}_2} = -\frac{\delta J}{\delta \hat{v}_2}, \quad \frac{1}{2\beta_2^2} (A \hat{v}_2, \hat{v}_2) = E;
\]

and, due to convexity of \( J(v) \), from 8.48) we have

\[
J(\hat{v}_1) - J(\hat{v}_2) \geq \left( \frac{\delta J}{\delta \hat{v}_2}, \hat{v}_1 - \hat{v}_2 \right).
\]

Therefore,

\[
\hat{S}_1(E) - \hat{S}_2(E) = 2\beta_1 E + J(\hat{v}_1) - (2\beta_2 E + J(\hat{v}_2)) =
\]

\[
= 2E(\beta_1 - \beta_2) + J(\hat{v}_1) - J(\hat{v}_2) \geq 2E(\beta_1 - \beta_2) + \left( \frac{\delta J}{\delta \hat{v}_2}, \hat{v}_1 - \hat{v}_2 \right) =
\]

\[
= 2E(\beta_1 - \beta_2) - \frac{1}{\beta_2^2} (A \hat{v}_2, \hat{v}_1 - \hat{v}_2) \geq 2E(\beta_1 - \beta_2) + \frac{1}{\beta_2^2} (A \hat{v}_2, \hat{v}_2) -
\]

\[
- \frac{1}{\beta_2^2} (A \hat{v}_2, \hat{v}_1) \geq 2E\beta_1 - \frac{1}{2|\beta_2^2|} \left( \alpha (A \hat{v}_1, \hat{v}_1) \right) + \frac{1}{\alpha} (A \hat{v}_2, \hat{v}_2) =
\]

\[
= 2E\beta_1 - \frac{E}{|\beta_2^2|} (\alpha \beta_1^2 + \frac{1}{\alpha} \beta_2^2) = 2E\beta_1 - 2E|\beta_1|.
\]

Here we choose the optimum value of an arbitrary constant \( \alpha \) to be \( |\beta_2/\beta_1| \).

So, if a solution of (8.44), (8.45) exists for positive \( \beta \), it is unique, and

this is the only solution we need; the values of entropy for negative \( \beta \) are smaller the one corresponding to the positive \( \beta \).

However, there are interesting cases when the solution for positive \( \beta \) does not exist, and only solutions for negative \( \beta \) (negative temperature states)
should be sought. This happens if the most probable value of energy is zero. Indeed, let the averaged functional $l_0(r)$ be zero:

$$\int l_0(r) f_0(r) \, dr = 0.$$  \hspace{1cm} (8.50)

Then equation (8.45) always have zero solution $\ddot{v} = 0$ for any $\beta$. Since the solution of (8.45) is unique for positive $\beta$, we have $\ddot{v} = 0$ for $\beta > 0$. This is inconsistent with equation (8.44) for $E > 0$. We conclude that $\beta$ should be negative if (8.50) holds.

The typical graphs of the dependence of entropy on energy are shown in Fig. 1. If the most probable value of energy, $\bar{E}$, is not zero, then both signs of temperature are possible since $\beta = dS(E)/dE$. Negative temperature corresponds to large values of energy. If the most probable value of energy, $\bar{E}$, is zero, temperature is always negative. In the example considered in Appendix C all eigenvalues $\beta$ are negative, and the maximum value of $\beta$ corresponds to the maximum value of entropy. It is not known at present whether this is a general feature of the entropy functional.

Some features of the entropy values follow from the inequality (8.49). Let us denote the only positive value of $\beta$ by $\beta_0$, and put all negative values of $\beta$ in decreasing order, $\beta_1 \geq \beta_2 \geq \beta_3...$ ($|\beta_1| \leq |\beta_2| \leq |\beta_3|...$). The corresponding values of entropy we denote by $S_0(E), S_1(E),...$. If there is a positive value of $\beta$, then, as we found from (8.49)

$$S_0(E) \geq S_k(E), \quad k = 1, 2, \ldots$$

Substituting in (8.49) $S_k$ and $S_m$ instead of $S_1$ and $S_2$ we obtain the estimation

$$S_k(E) \geq S_m(E) - 4E|\beta_k|, \quad m = 0, 1, 2, \ldots$$  \hspace{1cm} (8.51)

If the conjecture $S_k(E) \geq S_m(E)$ for $m > k$, is true, then only the cases $m < k$ in (8.51) yield nontrivial inequalities. They all are consequences of the strongest one,

$$S_k(E) \geq S_0(E) - 4E|\beta_k| \quad k = 1, 2, \ldots$$  \hspace{1cm} (8.52)

Similarly we obtain that, if there are no positive $\beta$, the strongest estimate is

$$S_k(E) \geq S_1(E) - 4E|\beta_k| \quad k = 2, \ldots$$  \hspace{1cm} (8.53)
Figure 1: Dependence entropy on energy: a) the most probable value of energy is not zero; b) the most probable value of energy is zero

There is a relation which allows one to better understand the meaning of function $\hat{v}$. Events $r_1, ..., r_N$ are distributed independently with probability density function $f_0(r)$. One may wonder what is the conditional probability density function of the first event, $\hat{f}(r)$, if one considers only the events $r_1, ..., r_N$ for which energy takes some given value $E$. It turns out that

$$\hat{f}(r) = \text{const} \times e^{-\langle t_0(r), \hat{v} \rangle} f_0(r). \quad (8.54)$$

Conditional probability density functions of $r_2, ..., r_N$ are the same.

A derivation of (8.54) is given in Appendix B.

Formula (8.54) explains the meaning of the stationary point of the entropy functional: the solution of (8.45), $\hat{v}$, is the solution of the original variational problem averaged over all events $r_1, ..., r_N$ for which energy has a given value, $E$.

9 The basic identity

The proof of the asymptotic formula (1.5) will be based on the following identity

$$f(E) = R e^N \hat{S} (E)$$

$$R = \tilde{M} \left[ e^{-\frac{\mathbb{S}(A^{-1}r, \hat{v})}{\hat{\mathbb{S}}}} \delta \left( \frac{\langle \hat{r}, \hat{v} \rangle}{\beta} + \frac{1}{2} (A^{-1} \hat{r}', \hat{r}') \right) \right] \quad (9.55)$$
where \( M \) is the mathematical expectation with respect to the auxiliary measure

\[
\tilde{f}(r) = e^{-\{\tilde{\alpha}(r), \tilde{\nu}\}} f_0(r) \int e^{-\{\alpha_0(r), \nu\}} f_0(r) dr ,
\]

(9.56)

the couple \((\beta, \tilde{\nu})\) is any solution of equations (8.44), (8.45), \( \ell' = l - \tilde{l}_0 \), \( \tilde{l}_0 \) is the average value of \( l \) with respect to the auxiliary measure,

\[
\tilde{l}_0 = \int l_0(r) \tilde{f}(r) dr ,
\]

(9.57)

and \( A^{-1} \) is the inverse operator for \( A \), i.e. for any \( l \)

\[
\min_u \left[ \frac{1}{2} (Au, u) - (l, u) \right] = \frac{1}{2} (A^{-1} l, l) .
\]

First, we give a derivation of (9.55) based on the identity (1.14). Actually, the author came to (1.5) and (9.55) using this line of reasoning. In the next section, another derivation of (9.55) is presented which is much simpler but could be hardly found before (9.55) was obtained in the long way described in this section.

Consider the following function of complex variable \( z \)

\[
\hat{f}(z) = M \left[ e^{z \min_u I(u, r)} \right] .
\]

By definition of probability,

\[
\hat{f}(z) = \int_0^{\infty} e^{-zE} f(E) dE .
\]

(9.58)

Here we used that energy does not make negative values. Thus, function \( \hat{f}(z) \) is the Laplace transform of the probability density function of energy, \( f(E) \). On the imaginary axis, \( z = iy \) \( \hat{f} \) coincides with the characteristic function. Since

\[
f(E) \geq 0 \quad \text{and} \quad \int_0^{\infty} f(E) dE = 1 ,
\]

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function \( \hat{f}(z) \) is analytic in the right half-plane, \( \Re z > 0 \). It tends to zero along each line, \( z = x_0 + iy, x_0 \) is fixed, \( |y| \to \infty \). Formula (9.55) can be inverted (see, for example, [16])

\[
f(E) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{Ez} \hat{f}(z)\,dz. \tag{9.59}
\]

Consider the scaled function,

\[
\hat{f}(Nz) = M \left[ e^{Nz \min_u I(u,r)} \right]. \tag{9.60}
\]

We expect that for large \( N \)

\[
\hat{f}(Nz) \approx e^{NB(z)}
\]

where \( B(z) \) is some function which is independent on \( N \). If this is the case, then, by changing the variable of integration \( z \) in (9.59) to \( Nz \), we arrive at the problem of studying the asymptotics of the integral,

\[
f(E) = \frac{N}{2\pi i} \int_{c-i\infty}^{c+i\infty} e^{N(Ez + B(z))} \,dz.
\]

This can be attempted by the steepest descent method. We will proceed this way.

The first step is to study the asymptotic behavior of the function \( \hat{f}(Nz) \) (9.60) for \( N \to \infty \). A natural desire is to make "a homogenization" in (9.60) by changing the order of minimization with respect to \( u \) and averaging with respect to \( r \). Fortunately, this is possible in the problems under consideration due to (1.14). We discuss first this identity in more details.

Consider a finite-dimensional variational problem when \( I(u,r) = \frac{1}{2} (Au,u) - (l(r),u) \)

is a quadratic function of a point \( u \) in \( m \)-dimensional space \( \mathbb{R}^m \), \( u = (u_1,\ldots,u_m) \), \( A \) is a positive \( m \times m \) matrix, \( (Au,u) \) is the corresponding positive quadratic form. By \( (l,u) \) we denote the scalar product of the vector \( l \) (which is a function of the event, \( r \)) and \( u \). We introduce also the vector \( \zeta = iu \) with pure imaginary components, \( \zeta_1 = iu_1,\ldots,\zeta_m = iu_m \). For complex-valued vectors, the scalar product used here does not contain the complex conjugation, for example: \( (l,\zeta) = i(l,u) \).
For any $z$, $\Re z > 0$, the following identity holds

$$
\frac{1}{i^m} \sqrt{\frac{z^m}{(2\pi)^m} \det A} \int_{-i\infty}^{i\infty} \cdots \int_{-i\infty}^{i\infty} e^{z\left[\frac{1}{2}(A\zeta, \zeta)-(l, \zeta)\right]} d^m \zeta = e^{-\frac{1}{2}z(A^{-1}l, l)}
$$

(9.61)

Here $d^m \zeta \equiv d\zeta_1, \ldots, d\zeta_n$ and $A^{-1}$ is the inverse of the matrix $A$. Formula (9.61) (written in terms of variable $u$) can be found, for example, in [7] (ch. 2, sec. 3). As was mentioned in Introduction, (9.61) can be written also in another form:

$$
e^{z \min_u \left[\frac{1}{2}(Au, u)-(l, u)\right]} = \frac{1}{i^m} \sqrt{\frac{z^m}{(2\pi)^m} \det A} \int_{-i\infty}^{i\infty} \cdots \int_{-i\infty}^{i\infty} e^{z\left[\frac{1}{2}(A\zeta, \zeta)-(l, \zeta)\right]} d^m \zeta.
$$

(9.62)

This means that the function which is the subject of averaging in (9.60) can be presented in the form of an integral of a function of auxiliary variables $\zeta$. Averaging is an integration over an event, $r$. The order of integration over $\zeta$ and over $r$ can be changed since the integrals converge absolutely. Thus we arrive at the expression:

$$
M \left[ e^{Nz \min_u I(u, r)} \right] = 
$$

$$= \frac{1}{i^m} \left( \frac{Nz}{2\pi} \right)^{m/2} \int_{-i\infty}^{i\infty} \cdots \int_{-i\infty}^{i\infty} M \left[ \sqrt{\det A} e^{Nz\left[\frac{1}{2}(A\zeta, \zeta)-(l, \zeta)\right]} \right] d^m \zeta.
$$

(9.63)

For weakly stochastic problems, only $(l, \zeta)$ is random. If $(l, \zeta)$ has the form (1.7) then

$$Me^{-Nz(l, \zeta)} = \left[ \int e^{-z(l_0(r), \zeta)} f_0(r) dr \right]^N
$$

and (9.63) takes the form

$$M \left[ e^{Nz \min_u I(u, r)} \right] =
$$

$$= \int_{-i\infty}^{i\infty} \cdots \int_{-i\infty}^{i\infty} \frac{1}{i^m} \left( \frac{Nz}{2\pi} \right)^{m/2} \det A e^{N\left[\frac{1}{2}(A\zeta, \zeta)+\ln \int e^{-z(l_0(r), \zeta)} f_0(r) dr \right]} d^m \zeta
$$

(9.64)
For the probability density function of energy we have

\[
f(E) = \frac{N}{2\pi^{m+1}} \int \sqrt{\left(\frac{Nz}{2\pi}\right)^{m}} \det A \ e^{NS} d^{m} \zeta dz;
\]

\[
S = Ez + \frac{z}{2}(A\zeta, \zeta) + \ln \int e^{-z(l_{0}(r),\zeta)} f(r) \, dr.
\]  \hspace{1cm} (9.65)

If a formal change of variables is made, \( \zeta \rightarrow \zeta/z \) then (9.65) takes the form

\[
f(E) = \frac{N}{2\pi^{m+1}} \int \sqrt{\left(\frac{Nz}{2\pi}\right)^{m}} \det A \ e^{NS} d^{m} \zeta dz;
\]

\[
S = Ez + \frac{1}{2z}(A\zeta, \zeta) + \ln \int e^{-z(l_{0}(r),\zeta)} f_{0}(r) \, dr.
\]  \hspace{1cm} (9.66)

In (9.66) the paths of integration for \( \zeta \) can be chosen again as the straight lines which are parallel to the imaginary axis. The direct derivation of this fact from (9.65) and (9.66) is cumbersome, and a better way is to choose another starting point instead of the identity (9.61), the analogous identity involving some arbitrary constants \( \alpha = (\alpha_{1}, \ldots, \alpha_{m}) \):

\[
e^{-\frac{1}{2}z(A^{-1}L)L} = \frac{1}{iz^{m}} \sqrt{\det A} \int_{-\infty}^{\infty} \ldots \int_{-\infty}^{\infty} e^{\frac{1}{2z}[(A\zeta, \zeta)-(L, L)]} d^{m} \zeta.
\]  \hspace{1cm} (9.67)

The identity (9.67) follows from (9.61) by the change of variables \( \zeta \rightarrow \zeta = \alpha + \zeta \) and \( l \rightarrow l - z^{-1}A\alpha \). In accordance with (9.67), (9.59) and (9.60), the relation (9.66) is true where the paths of integration in \( \zeta \)-planes are arbitrary straight lines which are parallel to the imaginary axis, while in \( z \)-plane this path should be in the right half-plane:

\[
f(E) = \frac{N}{2\pi^{m+1}} \int \int \ldots \int \sqrt{\left(\frac{Nz}{2\pi}\right)^{m}} \det A \ e^{NS} d^{m} \zeta dz.
\]  \hspace{1cm} (9.68)
Relation (9.68) suggests that $f(E)$ can be obtained by the steepest descent method. However, there is a difficulty.

Note that $m$ in (9.68) can be large, in the order of $N$, or even much larger than $N$: the number of basic functions needed for an accurate approximation of the functional $I(u, r)$ may be much larger that $N$. The steepest descent method was developed for the case when $m$ is fixed and $N \to \infty$, and, thus, cannot be applied to (9.68) directly. The fact that the standard steepest descent method does not work for $m >> N$ can be seen from the following example.

Consider a finite-dimensional truncation of the functional,

$$ S(u) = \int_0^1 u^2 \, dx. $$

Let us take the truncation of the form

$$ S_m(u) = \frac{1}{m} \sum_{k=1}^m u_k^2 $$

where $u_k$ are the values of function $u(x)$ at the points $k/m$. It is clear that the integral

$$ \int_{\mathbb{R}^m} e^{-N S_m(u)} \, dm_u = \left[ \int_{\mathbb{R}^m} e^{-\frac{N}{m} u^2} \, du \right]^m = \left( \sqrt{\frac{m}{2\pi N}} \right)^m $$

has different asymptotics depending on the relative order of $N$ and $m$. Slightly complicating this example we may observe that the asymptotics does not necessary relate to the minimum of $S(u)$.

Another difficulty in (9.68) is a study of stationary points of $S$ which is a function of many complex variables.

Thus, we proceed in a different way trying to get an identity for $f(E)$

which contains $e^{N S}$ as a factor, and evaluating in which cases this factor indeed determines the asymptotics of $f(E)$.

To this end we note that $\alpha$ in (9.68) can be some functions of $z$ and choose $((\beta, \bar{v})$ is the stationary point of $S(E, z, \zeta)$ with respect to $z, \zeta$).

$$ \alpha = \frac{z}{\beta} \frac{v}{\bar{v}}, \quad \kappa = \beta. $$

\footnote{In the derivation of this section $\beta$ is assumed to be positive. This is not required in the derivation of the next section.}
Then, putting $\zeta = \alpha + iv$ ($v$ is a vector in $R^n$) and $z = \beta + iy$, we have

$$S(E, z, \zeta) = Ez + \frac{1}{2z} (A\zeta, \zeta) + \ln \int e^{-(\ell_0(r, \zeta))} f_0(r) dr =$$

$$= Ez + \frac{1}{2z} \left[ \frac{z^2}{\beta^2} (A\bar{v}, \bar{v}) + 2 \frac{z}{\beta^2} (A\bar{v}, v) - (Av, v) \right] +$$

$$+ \ln \int e^{-(\ell_0(r, \bar{v}))} f_0(r) dr + \ln \int e^{-(\ell_0(r, \bar{v}))} f_0(r) dr. $$

where $\bar{f}$ is determined by (9.56). Since

$$(A\bar{v}, \bar{v}) = 2\beta^2 E, \quad \frac{1}{\beta} A\bar{v} = \bar{l}_0, \quad (\bar{l}_0, \bar{v}) = 2E\beta$$

the functional $S$ takes the form

$$S(E, z, \zeta) = \bar{v} + 2Eiy - \frac{1}{2z} (Av, v) + \frac{i}{\beta} (A\bar{v}, \bar{v}) + \ln \int e^{-(\ell_0, \bar{v})} \bar{f}(r) dr =$$

$$= S - \frac{1}{2z} (Av, v) + \ln \int e^{-(\ell_0, \bar{v} + v)} \bar{f}(r) dr.$$

So,

$$f(E) = Re^{N\bar{v}}$$

(9.69)

where

$$R = \frac{N}{2\pi} \int_{-\infty}^{+\infty} \sqrt{\left( N \frac{m}{2\pi \beta} \right)} \det A \ e^{-\frac{1}{2\pi} (Av, v) + \ln \int e^{-(\ell_0, \bar{v} + v)} \bar{f}(r) dr} \ d^m v dy. $$

(9.70)

The prefactor can be also put in another form using the transformation,

$$\int \sqrt{\left( N \frac{m}{2\pi \beta} \right)} \det A \ e^{-\frac{N}{2\pi} (Av, v) - \frac{1}{2\pi} (l, \bar{v})} \bar{f}(r) dr \ d^m v =$$

$$= \tilde{M} \int \sqrt{\left( N \frac{m}{2\pi \beta} \right)} \det A \ e^{-\frac{N}{2\pi} (Av, v) - \frac{1}{2\pi} (l, \bar{v})} \ d^m v =$$

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\[ M e^{-N i (\ell', \nu') \frac{1}{\beta} - \frac{N}{2} (A^{-1} \ell', \ell')} \]  

(9.71)

Since
\[ \int_{-\infty}^{+\infty} e^{-N i y \left[ \frac{1}{2} (\ell', \nu') + \frac{1}{2} (A^{-1} \ell', \ell') \right]} dy = \frac{2\pi}{N} \delta \left( \frac{1}{\beta} (\ell', \nu') + \frac{1}{2} (A^{-1} \ell', \ell') \right) , \]  

(9.72)

we arrive at (9.55).

Now we check (9.55) by the direct inspection.

10 Another derivation of the basic identity

First we present the probability density function of energy in the form
\[ f(E) = M \delta \left( E - \frac{1}{2} (A^{-1} \ell, \ell) \right) = \frac{N}{2\pi i} M \int_{-i\infty}^{+i\infty} e^{N \left[ E z - \frac{1}{2} (A^{-1} \ell, \ell) \right]} d\ell = \]

\[ \frac{N}{2\pi i} \int_{-i\infty}^{+i\infty} e^{N \left[ E z - \frac{1}{2} (A^{-1} \ell, \ell) \right]} f_0(\ell_1) \ldots f_0(\ell_N) d^N \ell \]  

(10.73)

Introducing averaging with respect to measure (9.56), and using (1.7) and the relation
\[ \mathcal{S} = E \beta + \frac{1}{2\beta} (A \mathcal{V}, \mathcal{V}) + \ln \int e^{-\{l_0, \mathcal{V}\}} f_0(\ell) d\ell = \]

\[ = 2E \beta + \ln \int e^{-\{l_0, \mathcal{V}\}} f_0(\ell) d\ell \]  

(10.74)

we can write
\[ f(E) = e^{N \mathcal{S}} \left( \frac{N}{2\pi i} M \right) \int_{-i\infty}^{+i\infty} e^{N \left[ E z - 2E \beta + (l(r), \mathcal{V}) - \frac{1}{2} (A^{-1} \ell, \ell) \right]} d\ell . \]  

(10.75)

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Changing in (10.75) \( l \) by \( \tilde{l}_0 + l' \) we have

\[
f(E) = e^{N \frac{s}{\beta}} \frac{N}{2\pi i} \bar{M} \int_{-i\infty}^{i\infty} e^{N\Delta S} dz;
\]

(10.76)

\[
\Delta S = Ez - 2E\beta + (\tilde{l}_0, \tilde{v}) + (l', \tilde{v}) - \frac{z}{2} (A^{-1}\tilde{l}_0, \tilde{l}_0) - z (A^{-1}l'_0, l') - \frac{z}{2} (A^{-1}l', l').
\]

(10.77)

Note that equation (8.45) takes a simple form in terms of measure (9.56):

\[
\frac{1}{\beta} A^\dagger \tilde{v} = \tilde{l}_0.
\]

(10.78)

Thus, in accordance with (8.44),

\[
(\tilde{l}_0, \tilde{v}) = 2\beta E, \quad (A^{-1}\tilde{l}_0, \tilde{l}_0) = \left( \frac{\tilde{v}}{\beta}, \tilde{l}_0 \right) = \frac{1}{\beta^2} (A^\dagger \tilde{v}, \tilde{v}) = 2E,
\]

\[
(A^{-1}l'_0, l') = \left( \frac{\tilde{v}}{\beta}, l' \right).
\]

(10.79)

Due to (10.79) some terms in (10.77) cancel out, and \( \Delta S \) is simplified to

\[
\Delta S = (l', \tilde{v}) - z \left( \frac{1}{\beta} (l', \tilde{v}) + \frac{1}{2} (A^{-1}l', l') \right).
\]

(10.80)

Integration over \( z \) in (10.76) gives \( \delta \)-function

\[
\frac{N}{2\pi i} \int_{-i\infty}^{i\infty} e^{N\left( \frac{z}{2} (l', \tilde{v}) + \frac{z}{2} (A^{-1}l', l') \right)} dz = \delta \left( \frac{1}{\beta} (l', \tilde{v}) + \frac{1}{2} (A^{-1}l', l') \right)
\]

and we arrived at (9.55).

11 An estimation of the prefactor

Let us find the limit behavior of the prefactor in (9.55),

\[
R = \bar{M} \left[ e^{-\frac{N\beta}{2} (A^{-1}l', l')} \delta \left( \frac{1}{\beta} (l', \tilde{v}) + \frac{1}{2} (A^{-1}l', l') \right) \right].
\]

(11.81)
To this end we make an \( m \)-dimensional projection of the space of functions \( u \). Then \( \ell' \) becomes an \( m \)-dimensional vector, while \( A^{-1} \) is the positive \( m \times m \) matrix. Vector \( \xi = \sqrt{N} \ell' \), as a sum of statistically independent similarly distributed vectors, has Gaussian distribution with the finite second moments

\[
B = \bar{M} \xi \otimes \xi = \bar{M} l_0 \otimes l_0 - (\bar{M} l_0) \otimes (\bar{M} l_0).
\]

(11.82)

Thus, up to small terms of the order \( N^{-1/2} \)

\[
R = \sqrt{\frac{\det B^{-1}}{(2\pi)^m}} \int e^{-\frac{\beta}{2} \langle A^{-1} \xi, \xi \rangle} \delta \left( \frac{1}{\beta \sqrt{N}} \langle \xi, \hat{v} \rangle + \frac{1}{2N} \langle A^{-1} \xi, \xi \rangle \right) e^{-\frac{1}{2}(B^{-1} \xi, \xi)} d^n \xi =
\]

\[
= \sqrt{\frac{\det B^{-1}}{(2\pi)^m}} \int e^{-\frac{1}{2}(C \xi, \xi)} \delta \left( \frac{1}{2N} \langle A^{-1} \xi, \xi \rangle + \frac{1}{\beta \sqrt{N}} \langle \xi, \hat{v} \rangle \right) d^n \xi,
\]

where

\[
C = B^{-1} + \beta A^{-1}
\]

Presenting \( \delta \)-function in terms of the Fourier integral we have

\[
R = \sqrt{\frac{\det B^{-1}}{(2\pi)^m}} \frac{1}{2\pi} \int e^{-\frac{1}{2}((C - \frac{\beta}{N} A^{-1}) \xi, \xi) + \frac{\beta}{\sqrt{N}} \langle \xi, \hat{v} \rangle} d^n \xi dt;
\]

\[
R = \frac{1}{2\pi} \int \sqrt{\frac{\det B^{-1}}{\det (C - \frac{\beta}{\sqrt{N}} A^{-1})}} e^{-\frac{1}{2}((C - \frac{\beta}{N} A^{-1}) \hat{v}, \hat{v})} \frac{t^2}{\beta^2} \frac{1}{dt}.\]

Changing the variable of integration \( t \rightarrow t \sqrt{N} \) we put \( R \) in the form

\[
R = \sqrt{N} \frac{1}{2\pi} \int \sqrt{\frac{\det B^{-1}}{\det (C - \frac{\beta}{\sqrt{N}} A^{-1})}} e^{-\frac{1}{2}((C - \frac{\beta}{N} A^{-1}) \hat{v}, \hat{v})} \frac{t^2}{\beta^2} dt. \quad (11.83)
\]

Assuming that there is a limit of \( \det B^{-1} / \det C \) for \( m \to \infty \), we see that the integral in (11.83) has the finite limit for \( N \to \infty \), and, in the first approximation,

\[
R = \sqrt{\frac{N \det B^{-1}}{2\pi \det C (\hat{v}, \hat{v})}} \beta
\]

This completes the justification of formula (1.5).
An estimation of the prefactor which does not use the Gaussian distribution of \( l' \) can be obtained from (9.70). Changing variables \( v \rightarrow \sqrt{2}v/\sqrt{N} \), \( y \rightarrow y/\sqrt{N} \) we have

\[
R = \frac{\sqrt{N}}{2\pi} \int_{-\infty}^{+\infty} \sqrt{\det A} e^{-\frac{1}{2}(Av,v)+\Phi_N(u)} d^m v dy
\]

(11.84)

\[
\frac{y}{v} = v + v\sqrt{z}, \quad z = \beta + i \frac{y}{\sqrt{N}}
\]

\[
\Phi_N(u) = N \ln \int e^{-\sqrt{\frac{1}{m} (k, u)}} f(r) dr
\]

(11.85)

Let

\[
\Phi_{\infty}(u) \equiv \lim_{N \to \infty} \Phi_N(u) = -\frac{1}{2}(Bu,u)
\]

(11.86)

and

\[
|e^{\Phi_N(u) - \Phi_{\infty}(u)} - 1| \leq \frac{1}{N^\sigma} (u,u)^{\kappa}, \quad \sigma > 0
\]

Then

\[
R = \frac{\sqrt{N}}{2\pi} \int_{-\infty}^{+\infty} \sqrt{\det A} e^{-\frac{1}{2}(Av,v)-\frac{1}{2}(Bu,u)} d^m v dy + R'
\]

(11.87)

\[
R = \frac{\sqrt{N}}{2\pi} \int_{-\infty}^{+\infty} \sqrt{\det A} e^{-\frac{1}{2}(Av,v)-\frac{1}{2}(Bu,u)} (e^{\Phi_N - \Phi_{\infty}} - 1) d^m v dy
\]

If the integral

\[
\int_{-\infty}^{+\infty} \sqrt{\det A} (u,u)^{\kappa} e^{-\frac{1}{2}(Av,v)-\frac{1}{2}(Bu,u)} d^m v dy
\]

converges and tends to some limit for \( N \to \infty, m \to \infty \), and the integral

\[
\int_{-\infty}^{+\infty} \sqrt{\det A} e^{-\frac{1}{2}(Av,v)-\frac{1}{2}(Bu,u)} d^m v dy
\]

(11.88)
has the limit for $m \to \infty$, $N \to \infty$, then $R' = O(1/N^\sigma)$ and the formula (1.5) is true. These conditions should be checked in each particular case. Note a necessary condition for the convergence of the integral (11.87): the limit

$$\lim_{m \to \infty} \sqrt{\frac{\det A}{\det (A + \beta B)}}$$

(11.89)

should exist and be finite and independent on $N$.

12 A counterexample.

The necessity of the existence of the finite limit (11.89) can be seen from the following example. Consider a 1D variational problem: the functional

$$I(u) = \frac{1}{2} \int_0^1 \left( \frac{du}{dx} \right)^2 dx - \int_0^1 \frac{du}{dx} \varepsilon(x) dx$$

(12.90)

takes its minimum value on the set of all $u(x)$ such that $u(0) = 0$. This is a problem of internal stresses in a beam with one clamped and one free edge, $\varepsilon(x)$ has the meaning of the residual strain. Let $\varepsilon(x)$ is a piece-wise function taking random independent values on the segments, $\left[ \frac{k-1}{N}, \frac{k}{N} \right]$ $k = 1, ..., N$.

For simplicity, we assume that $\varepsilon(x)$ takes the two values: $\varepsilon + \alpha$ with the probability $p_1$ and $\varepsilon - \alpha$ with the probability $p_2$ ($p_1 + p_2 = 1$). The minimum value of the functional (12.90) can be easily found:

$$L = -\frac{1}{2} \int_0^1 \varepsilon'^2 dx = -\frac{1}{2} \varepsilon^2 - \varepsilon \int_0^1 \varepsilon' dx - \frac{1}{2} \alpha^2$$

(12.91)

$\varepsilon'$ is the piece-wise function taking the values $\pm \alpha$. The random term in (12.91) has the form

$$\xi = \frac{1}{N} \sum_{k=1}^{N} \xi_k$$

(12.92)
where $\xi_k$ are independent random variables taking the value $\alpha$ with the probability $p_1$ and $-\alpha$ with the probability $p_2$. The probability density function, $f(\xi)$, of the random variable (12.92) can be determined by the steepest descent method from the exact formula

$$f(\xi) = \frac{N}{2\pi i} \int_{-i\infty}^{i\infty} e^{N(\xi z + \ln(p_1 e^{-z\xi} + p_2 e^{z\xi}))} dz$$  \hspace{1cm} (12.93)$$

which is obtained in the same way as (2.20) in section 3. We have

$$f(\xi) = \text{const} \times e^{N \hat{\xi}} S_1(\xi)$$  \hspace{1cm} (12.94)$$

where $\hat{\xi}$ is the stationary value of the function

$$S(\xi, z) = \xi z + \ln \left( p_1 e^{-z\xi} + p_2 e^{z\xi} \right)$$

One can check that the exact formula (12.94) does not coincide with the formula (1.5) written for the functional (12.90). The cause is that the limit (11.89) does not exist in the case under consideration. Indeed, the functional $\Phi_N$ (11.85) has the form (see also Appendix A)

$$\Phi_N(u) = \sum_k \ln \tilde{M} e^{-\int_0^s \left( \frac{du}{dx} \right)_k \left( \tilde{\xi} - \tilde{\xi} \right)_k}$$

where $\langle \cdot \rangle_k$ is the space averaging over $k$th segment:

$$\langle \cdot \rangle_k = \frac{1}{1/N} \int_{(k-1)/N}^{k/N} \cdot dx,$$

$\tilde{\xi}$ is the average value of $\tilde{\xi}$ with respect to the auxiliary measure, $(\tilde{\xi} - \tilde{\xi})_k$ is the value $\tilde{\xi} - \tilde{\xi}$ at the $k$th segment. For $N \to \infty$

$$\Phi_N(u) \to -\frac{1}{2N} a^2 \sum_{k=1}^N \left( \frac{du}{dx} \right)_k^2 = -\frac{1}{2} (Bu, u), \quad a^2 = \tilde{M} (\tilde{\xi} - \tilde{\xi})^2$$

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Function $\varepsilon = du/dx$ is a piece-wise function in this problem, thus

$$(Au, u) = \frac{1}{2N} \sum_{k=1}^{N} \varepsilon_k^2, \quad (Cu, u) = \frac{1}{N} a^2 \sum_{k=1}^{N} \varepsilon_k^2$$

and

$$\frac{\det A}{\det (A + BB)} = \frac{(1/N)^N}{\left[\frac{1}{N}(1 + \beta a^2)\right]^N} = e^{-N \ln(1 + \beta a^2)}$$

Hence, the prefactor makes the contribution in (1.5) of the same order as $\exp[N \hat{S}]$.

13 Large excitations

Consider now the case of the linear functional of the form

$$(l, u) = \frac{1}{\sqrt{N}} \sum_{i=1}^{N} (l_0(r_i), u)$$  \hspace{1cm} (13.95)$$

Average value of each member of the sum (13.95) should be zero since the average value of energy is assumed to be finite,

$$\int l_0(r)f_0(r)dr = 0$$  \hspace{1cm} (13.96)$$

As in the case of negative temperature states, some eigenvalue problem plays the key role in the analysis. For functionals of the form (13.95) this is the problem

$$A\varphi_k = \lambda_k B\varphi_k$$  \hspace{1cm} (13.97)$$

where the positive operator $Bu$ is determined by the condition

$$M(l_0, u)^2 = (Bu, u)$$

We assume that the eigenvectors $\{\varphi_k\}$ form a basis in the space of functions $u$, all eigenvectors are simple, and $\lambda = 0$ is not an eigenvalue. Obviously, all $\lambda_k$ are positive. Eigenfunctions are normalized by the condition

$$(B\varphi_i, \varphi_j) = \delta_{ij}$$
Then

\[ (A \varphi_i, \varphi_j) = \lambda_i \delta_{ij} \]

Two cases should be distinguished:

\[
\sum_{k=1}^{\infty} \frac{1}{\lambda_k} < +\infty \quad \text{and} \quad \sum_{k=1}^{\infty} \frac{1}{\lambda_k} = \infty \quad (13.98)
\]

We show that in the first case the probability density function is given by the formula

\[
f(E) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \frac{e^{Ez}}{\sqrt{\Phi(z)}} \, dz \quad (13.99)
\]

where \( \Phi(z) \) is an analytic function,

\[
\Phi(z) = \prod_{k=1}^{\infty} \left( 1 + \frac{z}{\lambda_k} \right) \quad (13.100)
\]

Moving the contour of integration to the both sides of the negative \( x \)-axis we transform the integral (13.101) into a fast converging series

\[
f(E) = \sum_{\text{odd } k=1}^{\infty} \frac{\sqrt{\lambda_k \lambda_{k+1}}}{\pi} e^{-\lambda_{k+1}E} \int_{0}^{\lambda_{k+1} - \lambda_k} \frac{e^{Ex}}{\sqrt{x(\lambda_{k+1} - \lambda_k - x)}} \, dx \quad (13.101)
\]

In the second case (13.98), the average value of energy is infinite, as can be observed by direct inspection, and the variational problem should be regularized. We consider the following regularization:

\[
I(u) = \lim_{m \to \infty} \left( \frac{1}{2} (Au, u)_m - (l, u)_m + \frac{1}{2} \sum_{k=1}^{m} \frac{1}{\lambda_k} \right) \quad (13.102)
\]

where \((Au, u)_m\) and \((l, u)_m\) are \(m\)-dimensional projections of the corresponding functionals. Then the probability density function of the functional (13.102) is given by (13.99) where function \( \Phi(z) \)

\[
\Phi(z) = \prod_{k=1}^{\infty} \left( 1 + \frac{z}{\lambda_k} \right) e^{-z/\lambda_k} \quad (13.103)
\]

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Derivation of (13.99), (13.100) is based on the identity (9.67). As before, making $m$-dimensional truncation of $I(u)$ we have

$$ f(E) = M\delta \left( E + \min_u I(u) \right) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{Ez} M e^{z\min_u I(u)} \, dz = $$

$$ = \lim_{m \to \infty} \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{Ez} \frac{1}{i^m} \sqrt{\det A} \frac{1}{(2\pi z)^m} M e^{\frac{1}{2}(A\zeta, \zeta) - \frac{1}{2}(I, \zeta)} \, d^m\zeta \, dz = $$

$$ = \lim_{m \to \infty} \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{Ez} \frac{1}{i^m} \sqrt{\det A} \frac{1}{(2\pi z)^m} e^{\frac{1}{2}(A\zeta, \zeta) + N \ln f \, e^{-\sqrt{\frac{1}{2}(E_0(r), \zeta)}} f_0(r)dr} \, d^m\zeta \, dz $$

(13.104)

Function

$$ N \ln \int e^{-\sqrt{\frac{1}{2}(E_0(r), \zeta)}} f_0(r)dr $$

tends for $N \to \infty$ to

$$ \frac{1}{2}(B\zeta, \zeta) $$

Substituting the limit value of this function in (13.104) we get

$$ f(E) = \lim_{m \to \infty} \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{Ez} \frac{1}{i^m} \sqrt{\det A} \frac{1}{(2\pi z)^m} e^{\frac{1}{2}(A\zeta, \zeta) + \frac{1}{2}(B\zeta, \zeta)} \, d^m\zeta \, dz = $$

$$ = \frac{1}{2\pi i} \int_{-\infty}^{\infty} e^{Ez} \lim_{m \to \infty} \sqrt{\det A} \frac{1}{\det(A + zB)} \, dz $$

(13.105)

In the basis $\{ \varphi_k \}$, the matrix $B$ is the unit matrix while $A$ is a diagonal matrix with the diagonal elements $\lambda_1, \lambda_2, \ldots$.

Thus,

$$ \lim_{m \to \infty} \frac{\det(A + zB)}{\det A} = \Phi(z) $$

and (13.105) coincides with (13.99). Formula (13.99) with the regularized function $\Phi(z)$ for the case of diverging series $\sum \lambda^{-1}$ can be obtained in the same way.

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14 Appendices

Appendix A. The basic identity for the linear functional (1.3)

The basic identity (9.55) has been proven for linear functionals of the form (1.7). Let us show that it remains the same in the case of the linear functionals (1.3).

Euler’s equations for the functional $S(1.6)$ are

$$A^\varphi u = \frac{1}{N} \sum_{i=1}^{N} \frac{\int e^{-\beta t_{i}(r)} l_{i}(r) f_{0}^{i}(r) dr}{\int e^{-\beta t_{i}(r)} f_{0}^{i}(r) dr} \quad (A.1)$$

$$E + \frac{1}{2} (A^\varphi u, \varphi u) - \frac{1}{N} \sum_{i=1}^{N} \frac{\int e^{-\beta t_{i}(r)} l_{i}(r) f_{0}^{i}(r) dr}{\int e^{-\beta t_{i}(r)} f_{0}^{i}(r) dr} = 0 \quad (A.2)$$

Taking the scalar product of (A.1) with $\varphi u$, we see that the last term in (A.2) is equal to $-(A^\varphi u, \varphi u)$. Thus, equation (A.2) can be written also as

$$E = \frac{1}{2} (A^\varphi u, \varphi u) \quad (A.3)$$

The stationary value of $S(E, z, u)$ is

$$\bar{S}(E) = 2E\beta + \frac{1}{N} \sum_{i=1}^{N} \ln Q_{i}$$

$$Q_{i} = \int e^{-\beta t_{i}(r)} f_{0}^{i}(r) dr \quad (A.4)$$

We introduce an auxiliary probabilistic measure

$$\tilde{f}_{0}^{i}(r) = \frac{e^{-\beta t_{i}(r)} \varphi u}{Q_{i}} f_{0}^{i}(r) \quad (A.5)$$

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and denote by $\tilde{l}_i$ the functional averaged with respect to this measure,

$$\tilde{l}_i = \int l_i(r) \tilde{f}_0(r) dr$$  \hspace{1cm} (A.6)

In these terms equation (A.1) takes a simple form:

$$A \overset{\vee}{u} = \frac{1}{N} \sum_{i=1}^{N} \tilde{l}_i \equiv \tilde{l}$$  \hspace{1cm} (A.7)

Denote by $l'_i$ the difference $l_i - \tilde{l}$ and by $(l', u)$ the functional

$$(l', u) = \frac{1}{N} \sum_{i=1}^{N} (l'_i, u)$$

Our goal is to prove that

$$f(E) = e^{N \overset{\vee}{S}} M \left[ e^{-\frac{N}{2} \delta(A^{-1} l', l')} \delta((l', \overset{\vee}{u}) + \frac{1}{2}(A^{-1} l', l')) \right]$$  \hspace{1cm} (A.8)

As in (10.73)

$$f(E) = M \delta(E - \frac{1}{2}(A^{-1} l, l)) = \frac{N}{2\pi i} M \int_{-i\infty}^{i\infty} e^{N[Ez - \frac{\overset{\vee}{S}}{2\beta}(A^{-1} l, l)]} dz =$$

$$= e^{N \overset{\vee}{S}} \frac{N}{2\pi i} M \int_{-i\infty}^{i\infty} e^{N[Ez - 2E\beta + \beta \frac{1}{N} \sum_{i=1}^{N} (l_i, \overset{\vee}{u}) - \frac{\overset{\vee}{S}}{2\beta}(A^{-1} l, l)]} dz =$$

$$= e^{N \overset{\vee}{S}} \frac{N}{2\pi i} M \int_{-i\infty}^{i\infty} e^{N[Ez - 2E\beta + \beta(l_i, \overset{\vee}{u}) - \frac{\overset{\vee}{S}}{2\beta}(A^{-1} l, l)]} dz$$

Here $\bar{M}$ is the mathematical expectation with respect to the auxiliary measure. Changing $l$ by $\tilde{l} + l'$ we have the following expression in the exponent

$$Ez - 2E\beta + \beta(l, \overset{\vee}{u}) + \beta(l', \overset{\vee}{u}) - \frac{z}{2}(A^{-1} l, l) - z(A^{-1} \tilde{l}, l') - \frac{z}{2}(A^{-1} l', l')$$  \hspace{1cm} (A.9)
From (A.3) and (A.7),
\[
\langle \tilde{l}, \tilde{u} \rangle = (A \tilde{u}, \tilde{u}) = 2E, \quad \frac{z}{2}(A^{-1} \tilde{l}, \tilde{l}) = \frac{z}{2}(\tilde{u}, \tilde{l}) = zE
\]
and (A.9) simplifies to
\[
\beta(l, \tilde{u}) - z(\tilde{u}, l) - \frac{z}{2}(A^{-1} l, l)
\]
Thus,
\[
f(E) = e^{N \frac{\gamma}{2} M} \frac{N}{2\pi i} \int_{-\infty}^{i\infty} e^{N \beta(f', \tilde{u}) - z(f, \tilde{u}) - \frac{z}{2}(A^{-1} f, f')} dz =
\]
\[
= e^{N \frac{\gamma}{2} M} \left[ e^{N \beta(f', \tilde{u})} \delta((\tilde{u}, l') + \frac{1}{2}(A^{-1} f', l')) \right]
\]
This is equivalent to (A.8).

The modified expression for the prefactor corresponding to (9.70) is
\[
R = \frac{N}{2\pi} \int_{-\infty}^{+\infty} \sqrt{\left( \frac{N}{2\pi z} \right)^m \det A} e^{\frac{N}{2 \beta} (Av, v) + \frac{1}{2} \sum_k A_k e^{-i(k \cdot v)} \delta_A dr} d^n v dy
\]

**Appendix B. An outline of the derivation of (8.54)**

Conditional probability density of the \( r_1 \) to be in the vicinity \( A \) of the point \( x \) while energy takes values between \( E \) and \( E + \Delta E \) is

\[
\text{meas} \{ r_1, r_2, ..., r_N : E \leq -\min_u \left[ \frac{1}{2} (Au, u) - \frac{1}{N} (l_0(r_1), u) - \frac{1}{N} \sum_{i=2}^{N} (l_0(r_i), u) \right] \leq E + \Delta E, r_1 \in A \} / \text{meas} \{ r_1, r_2, ..., r_N : E \leq -\min_u I(u, r) \leq E + \Delta E \}
\]

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If $\Delta E \to 0, A \to x$ then the numerator tends to

$$\text{const} \times e^{N\tilde{S}_1(E, x, N)} \Delta E f_0(x)$$

where $\tilde{S}_1(E, x, N)$ is the minimum stationary value of the functional

$$S_1(E, z, v, x, N) = E z + \frac{1}{2z}(A v, v) - \frac{1}{N}(l_0(x), v) + \ln \int e^{-(l_0(r), v)} f_0(r) dr$$

while the denominator is $\text{const} \times e^{N\tilde{S}_1(E)} \Delta E$. The functional (B.1) depends on small parameter $N^{-1}$ and can be studied by variational-asymptotic method [1]. In first approximation, as it is easy to see,

$$\tilde{S}_1(E, x, N) = \tilde{S}(E) - \frac{1}{N}(l_0(x), \tilde{v})$$

(B.2)

There are other terms of order $N^{-1}$ in (B.2), but they do not depend on $x$. Thus, keeping only the terms depending on $x$, we obtain

$$\tilde{f}(x) = \text{const} \times e^{-(l_0(x), \tilde{v})} f_0(x)$$

as claimed.

**Appendix C. Negative temperature states in a 1D problem**

Solution of equation (8.45) in case of negative temperatures is a nonlinear eigenvalue problem. It is hard to expect an exact solution to this equation. There are, however, exceptions: 1D problems. Here we consider the problem of minimization of the following functional:

$$I(u) = \frac{1}{2} \int_0^1 \left( \frac{du}{dx} \right)^2 dx - \frac{1}{2N} \sum_{i=1}^N (u(r_i) - u(r_{N+i}))$$

(C.1)

At the ends $u(x)$ is assumed to be zero. The minimizing function $\tilde{u}$ can be interpreted, for
example, as the string lateral displacement caused by $2N$ forces of small amplitude $1/2N$ applied at random points; the points are homogeneously and independently distributed over the string; each force has a counter-part with the opposite direction. The average value of the work done by the forces (the linear functional in (C.1)) is zero. Thus, the most probable value of energy is zero, and only negative values of temperature are relevant. The entropy functional has the form

$$S(E, z, v) = Ez + \frac{1}{2z} \int_0^1 \left( \frac{dv}{dx} \right)^2 dx + \frac{1}{2} \ln Q_1 + \frac{1}{2} \ln Q_2$$  \hspace{1cm} (C.2)$$

$$Q_1 = \int_0^1 e^{-v} dx, \quad Q_2 = \int_0^1 e^v dx,$$

$$v(0) = v(1) = 0$$  \hspace{1cm} (C.3)$$

The Euler equations of the entropy functional are

$$-\frac{1}{\beta} \frac{d^2v}{dx^2} - \frac{1}{2Q_1} e^{-v} + \frac{1}{2Q_2} e^v = 0$$  \hspace{1cm} (C.4)$$

$$E = \frac{1}{2\beta^2} \int_0^1 \left( \frac{dv}{dx} \right)^2 dx$$  \hspace{1cm} (C.5)$$

We drop here and in what follows the sign $\nabla$.

Integrating equation (C.4) over $x$ we obtain that the derivative of $v$ is periodic

$$\frac{dv}{dx}(0) = \frac{dv}{dx}(1)$$  \hspace{1cm} (C.6)$$

Therefore, it is reasonable to search for periodic solutions of equation (C.4) with periodic derivatives. If $v(x)$ is such a solution, that, as follows from (C.4), $v(x + c) + b$ is also a solution for any constants $c$ and $b$. Knowing $v(x)$, one can construct a one-parametric family of solutions of the original problem

$$v(x + c) - v(c)$$  \hspace{1cm} (C.7)$$

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which are equal to zero at both ends for any constant c. Of course, the entropy functional has the same value for each member of the family (C.7). The above mentioned non-uniqueness of the stationary points is caused by the symmetry of the entropy functional under transformations

\[ v(x) \rightarrow v(x + c) + b \]

on the set of all periodic functions \( v(x) \) with the period 1.

Multiplying (C.4) by \( dv/dx \) and integrating we have

\[
\frac{1}{2b} \left( \frac{dv}{dx} \right)^2 + \frac{1}{2Q_1} e^{-v} + \frac{1}{2Q_2} e^{v} = A = \text{const} \tag{C.8}
\]

Here \( b \equiv -\beta > 0 \). We seek for periodic solutions of (C.8) with periodic derivatives. If \( v(x) \) is a solution, then one can make a shift, \( v \rightarrow v' = v + c \) and choose \( c \) in such a way, that \( Q_1(v') = Q_2(v') \). Therefore, without loss of generality one can set \( Q_1 = Q_2 \equiv Q \). Changing the constant \( A \) by the constant \( A \equiv aQ \) we have

\[
\left( \frac{dv}{dx} \right)^2 = \frac{2b}{Q} (a - \cosh v) \tag{C.9}
\]

In the phase plane \((v, dv/dx)\) the integral curves form a family of the closed curves surrounding the origin. The dependence of \( v \) on \( x \) can be found from (C.9).

\[
\int \frac{dv}{\pm \sqrt{a - \cosh v}} = \sqrt{\frac{2b}{Q}} x \tag{C.10}
\]

The path of integration rotates around the origin a number of times, \( n \). For given \( n \) and \( b \), the value of parameter \( a \) is determined by the conditions

\[
\int_{v_{\text{max}}}^{v_{\text{min}}} \frac{dv}{\pm \sqrt{a - \cosh v}} = 4n \int_{0}^{v_{\text{min}}} \frac{dv}{\sqrt{a - \cosh v}} = \sqrt{\frac{2b}{Q}} \tag{C.11}
\]

\[
Q = \int_{0}^{1} e^{-v} dx = \int_{0}^{1} \cosh v \; dx = \int_{0}^{v_{\text{max}}} \cosh v \; dv = 4n \sqrt{\frac{2b}{Q}} \int_{0}^{v_{\text{min}}} \frac{\cosh v \; dv}{\pm \sqrt{a - \cosh v}} \tag{C.12}
\]
\[ a \equiv \cosh v_{\text{max}} \]

Equation (C.5) provides the link between energy and temperature: from (C.5) and (C.9)

\[
E = \frac{1}{2b^2} \int_0^{v_{\text{max}}} \left( \frac{dv}{dx} \right)^2 dx = \frac{1}{bQ} (a - Q)
\]

(C.13)

The integral appeared can be expressed in terms of elliptic integral \( F(t, k) \) and associated Legendre functions \(^2 P^0_\nu(a)\):

\[
\int_0^{v_{\text{max}}} \frac{dv}{\sqrt{a - \cosh v}} = \frac{\pi}{\sqrt{2}} P^0_\nu(a)
\]

\[
\int_0^{v_{\text{max}}} \frac{\cosh v dv}{\sqrt{a - \cosh v}} = \frac{\pi}{\sqrt{2}} P^0_\nu(a)
\]

\[
\int_0^{v_{\text{max}}} \frac{dv}{\sqrt{a - \cosh v}} = \frac{2}{\sqrt{a + 1}} \left[ F \left( \frac{\pi}{2}, \sqrt{\frac{a - 1}{a + 1}} \right) - F \left( t, \sqrt{\frac{a - 1}{a + 1}} \right) \right]
\]

Finally, for given \( E \) and \( N \), the values of \( b, Q, \) and \( a \) are determined from the system of nonlinear equations:

\[
b = 4n^2 \pi^2 P^0_{-1/2}(a) P^0_{1/2}(a), \quad Q = P^0_{1/2}(a)/P^0_{-1/2}(a), \quad E = \frac{1}{b} \left( \frac{a}{Q} - 1 \right)
\]

(C.14)

The corresponding value of entropy is equal to

\[ S(E) = -2E b + \ln Q \]

temporarily out

Fig. 2 shows the dependence of entropy and inverse temperature on energy for the first branch, \( n = 1 \). Note that the energy values are bounded above.

\(^2\)Note a misprint in 2.464.32 of [9]: the sign in the right hand side must be changed.
Figure 2: Dependence of entropy (a) and negative inverse temperature (b) on energy for the first branch, $n = 1$

Figure 3: Dependence of entropy (a) and negative inverse temperature (b) on energy for the second branch, $n = 2$

A numerical value of the upper limit is 0.03. Study of the asymptotics of the solution of equations (C.14) for $a \to \infty$ gives the asymptotic maximum value of energy $1/32n^2$, and very slow approaching of entropy to negative infinity, $S \approx -\ln \ln a$. Thus, the entropy decay is not seen on the Figures. The inverse temperature goes to infinity at the maximum value of energy.

Similar graphs for the second branch are plotted in Fig. 3a,b.

The dependence of entropy on energy in vicinity of zero is presented on Fig. 4 for the first five branches. The maximum entropy corresponds to the first branch. Entropy of each next branch is smaller than the entropy of previous one.

To provide small values of energy, the points of application of external
Figure 4: Dependence of entropy on energy for the first five branches

Figure 5: Probability density function of positions of positive (a) and negative (b) force for small $E = 0.000125$

Figure 6: Probability density function of positions of positive (a) and negative (b) force for $E = 0.0012$
Figure 7: Probability density function of positions of positive (a) and negative (b) force for $E = 0.0075$

Figure 8: Probability density function of positions of positive (a) and negative (b) force for $E = 0.02$

Figure 9: Probability density function of positions of positive (a) and negative (b) force for $E = 0.025$
forces must be almost homogeneously distributed over the beam. The probability density function of distribution of "positive" force is shown in Fig. 5a for $E = 0.000125$. The corresponding distribution of "negative" force is shifted to the right for $x = 0.5$ (Fig. 5b). It is seen formation of zones of localization, the regions where application of the external forces is more probable. The first branch has two localization zones. Of course, both zones can be translated along the string due to the above-mentioned periodicity.

Fig. 6a,b presents probability density functions of points of application of positive and negative forces for the value of energy $E = 0.0012$. Probability density functions for larger values of energy $E = 0.0075, 0.02, 0.025$ are shown in Figs. 7a,b, 8a,b and 9a,b.

Other branches have more localization zones. The $n$th branch has $2n$ localization zones. Qualitatively, the dependence of the size of the zones on energy is the same as for the first branch.

References

References


