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Phase Transition in an Interacting Bose System. An Application of the Theory of Ventsel' and Freidlin

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We consider a system of N bosons on a complete graph with V vertices interacting through hard core repulsion. With the use of the Ventsel'–Freidlin large-deviation theory of random perturbation of dynamical systems, we calculate the canonical free energy in the thermodynamic limit and prove that the system exhibits a phase transition.

KEY WORDS: Base–Einstein statistics; large deviations; phase transition.

1. INTRODUCTION

Since its discovery in the mid 1920s, Bose–Einstein condensation has been one of the major challenges of statistical physics. The interest was mainly motivated by London's[(15,16)] proposal according to which the superfluid phase transition of ^{4}He is actually a Bose–Einstein condensation.

Since then a lot of work has been done. The phase transition of the ideal Bose gas is well understood. For a fairly general and exhaustive treatment see ref. 1. But the influence of initerparticle interaction on the Bose–Einstein condensation remained essentially unexplained. To our knowledge, all the existing results refer to approximate models defined after some kind of ad hoc "momentum space diagonalization" (e.g., refs. 2–4, 12, and 17). (However, there are some one-dimensional exceptions: the one-dimensional Bose gas with δ-repulsion treated rigorously with the help of the Bethe ansatz in refs. 14 and 7. But this one-dimensional system does not exhibit a phase transition at finite temperature. In ref. 6 some very

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specially chosen boundary conditions are responsible for the phase transition.) Although these results are intuitively appealing and the mathematical tools involved are very attractive, they do not give a satisfactory answer to the following basic question: do interacting bosons ever condense?[13]

In the present paper we propose and solve rigorously (without any kind of "momentum space approximation") the following model of interacting bosons: the "space" of the system is a complete graph on V vertices and, accordingly, the one-particle Hamiltonian (i.e., the "kinetic energy operator") is the properly normalized discrete Laplacian on this graph. The interaction between the particles is hard-core repulsion. That is: at most one particle is allowed at any site of the graph (for definition of the model see Section 2). After some standard and one tricky random walk reductions, we reformulate the problem of the canonical thermodynamic limit as a genuine large-deviation problem associated with a family of inhomogeneous random walks on $\mathbb{Z}$ (Section 3) and we find that the theory of Freidlin and Ventsel' of random perturbations of dynamical systems[10,19,20,22,23] is designed exactly for this kind of problem (Section 4). The last three sections (Sections 5–7) are devoted to the analysis of the variational problem which arises from the Friedlin–Ventsel'-type formulation. This completes the calculation of the cannonical free energy and the proof that the system exhibits a nontrivial phase transition.

In our opinion, the interest of this paper is twofold. (1) As far as we know, for the first time a phase transition is proved for an interacting Bose system without ad hoc approximations. (But of course we admit that the fact that the model has no proper spatial structure is a serious drawback.) (2) From the point of view of the probabilist, we hope, it is a nice application of Friedlin and Ventsel's theory to a problem which arises naturally from mathematical physics.

After the presentation of a preliminary version of this result, Oliver Penrose indicated a completely different way of treating this model. His results, including an explicit formula for the amount of condensate, will be presented elsewhere.[18]

2. THE MODEL AND THE MAIN RESULT

We consider the canonical ensemble for N bosons on a complete graph on V vertices $\Lambda_V = \{1, 2, \dots, V\}$, interacting via hard-core repulsion. More exactly: the one-particle Hilbert space is V-dimensional:

$$\mathscr{H}_V = \{\varphi(x) \mid x \in \Lambda_V\}$$

and the one-particle Hamiltonian (or kinetic energy operator) is the properly normalized discrete Laplacian on the complete graph on Λ_V:

$$K_V \varphi(x) = -\Delta_V \varphi(x) = \frac{1}{V} \sum_{y \in \Lambda_V} (\varphi(x) - \varphi(y))$$

This operator is the orthogonal projection to the subspace orthogonal to the constant functions. Since the spectrum of K_V consists of two points $\{0, 1\}$, where 1 is $(V-1)$-fold degenerate, the statistical physics of noninteracting particles on this graph is quite trivial [see formulas (2.2), (2.3)].

The interaction considered is hard-core repulsion; i.e., formally,

$$U(x_1, \dots, x_N) = \begin{cases} 0 & \text{if} \quad i \neq j \Rightarrow x_i \neq x_j \\ \infty & \text{otherwise} \end{cases}$$

Our final aim is the calculation of the canonical free energy per unit volume

$$\beta f(\rho, \beta) = - \lim_{\substack{N, V \to \infty \\ N/V \to \rho}} \frac{1}{V} \log Z(\beta, N, V) \tag{2.1}$$

with the canonical partition function Z defined as

$$Z(\beta, N, V) = \mathrm{Tr}_B \exp(-\beta H_{V,N})$$

where Tr_B stands for the trace on the symmetric subspace of the N-fold tensor product $\mathscr{H}_V \otimes \cdots \otimes \mathscr{H}_V$, $H_{V,N}$ is the total Hamiltonian

$$H_{V,N} = H^0_{V,N} + U$$

$H^0_{V,N}$ is the Hamiltonian of the noninteracting bosons, ρ is the density, and β is the inverse temperature of the system.

For sake of comparison we give the (straightforward) results for the noninteracting system:

$$\beta f_{0,B}(\rho, \beta) = \begin{cases} -(\rho+1)\log(\rho+1) + \rho \log \rho + \beta\rho \\ \qquad \text{if} \quad \rho < \rho_{0,c} = \dfrac{1}{e^\beta - 1} \\ -(\rho_{0,c}+1)\log(\rho_{0,c}+1) + \rho_{0,c} \log \rho_{0,c} + \beta\rho_{0,c} \\ \qquad \text{if} \quad \rho \geqslant \rho_{0,c} \end{cases} \tag{2.2}$$

for Bose–Einstein statistics, and

$$\beta f_{0,\mathrm{F}}(\rho, \beta) = \rho \log \rho + (1-\rho) \log(1-\rho) + \beta\rho \tag{2.3}$$

for Fermi–Dirac statistics.

Thus, the free Bose gas exhibits a phase transition (i.e., Bose–Einstein condensation) (This is actually a very simple mean-field result.) The question is: how does the repulsive interaction influence this behavior? The answer is formulated as follows as the main result of this paper.

Theorem 1. The thermodynamic limit (2.1) exists for all values of $\rho \in [0, 1]$ and $\beta \in [0, \infty)$. The free energy per unit volume is given by

$$\beta f(\rho, \beta) = \rho \log \rho + (1-\rho)\log(1-\rho) + \beta\rho + \begin{cases} 0 & \text{if} \quad 0 \leqslant \beta < \beta_{\mathrm{cr}} \\ \dfrac{(1-2\rho)^2}{2}(\beta - \beta_{\mathrm{cr}}) + \dfrac{1}{2}\log[1 - E(\beta)] + \rho(1-\rho)\,\beta E(\beta) \\ \quad \text{if} \quad \beta_{\mathrm{cr}} \leqslant \beta \end{cases} \tag{2.4}$$

where

$$\beta_{\mathrm{cr}} = \beta_{\mathrm{cr}}(\rho) = \frac{1}{1-2\rho} \log \frac{1-\rho}{\rho} \in (0, \infty) \tag{2.5}$$

and $E(\beta) \in [0, 1)$ is the unique solution of the equation

$$\frac{1}{[(1-2\rho)^2 + 4\rho(1-\rho)E]^{1/2}} \log \frac{1 + [(1-2\rho)^2 + 4\rho(1-\rho)E]^{1/2}}{1 - [(1-2\rho)^2 + 4\rho(1-\rho)E]^{1/2}} = \beta \tag{2.6}$$

Remarks. 1. Observe that the left-hand side of (2.6), as a function of $E \in [0, 1)$, is C_∞ and strictly increasing, taking the value $\beta_{\mathrm{cr}}(\rho)$ for $E = 0$ and having the limit $+\infty$ as $E \to 1$.

2. This system of interacting bosons exhibits a phase transition at the inverse temperature $\beta_{\mathrm{cr}}(\rho)$. It is easy to check that the functions $\beta \mapsto f(\rho, \beta)$ and $\beta \mapsto (\partial f/\partial\beta)(\rho, \beta)$ are continuous, while the map $\beta \mapsto (\partial^2 f/\partial\beta^2)(\rho, \beta)$ has a jump discontinuity at $\beta = \beta_{\mathrm{cr}}(\rho)$. The graph of the heat capacity as a function of temperature at fixed density is shown in Fig. 1. The jump in the heat capacity is

$$C(T_{\mathrm{cr}} - 0) - C(T_{\mathrm{cr}} + 0) = \left(\log \frac{1-\rho}{\rho}\right)^2 \left(\frac{1}{\rho(1-\rho)} - \frac{2}{1-2\rho} \log \frac{1-\rho}{\rho}\right)^{-1}$$

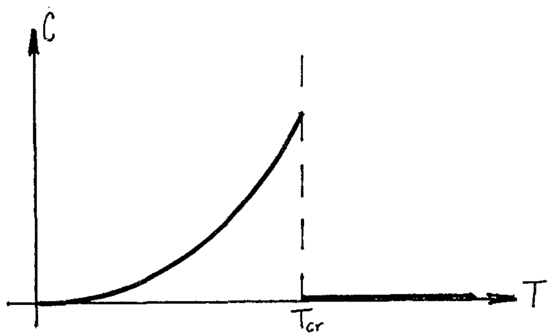

Fig. 1. The heat capacity as a function of temperature.

3. It is worth observing that above the critical temperature the free energy coincides with the free energy of the noninteracting fermion system on the same graph [compare (2.3) and (2.4)]. Is this a general property of hard-core boson systems on graphs? This conjecture is supported by the results in ref. 10 and 14 besides ours.

The rest of this paper is devoted to the proof of Theorem 1.

3. RANDOM WALK REPRESENTATIONS

As the one-particle free Hamiltonian is the generator of a continuous-time random walk on the complete graph on Λ_V with total jump rate $(V-1)/V$, we can use the basic random walk representation of the partition function (i.e., a Feynman–Kac formula). Let $\mathscr{P}_{x_1, x_2,..., x_N}$ be the joint probability distribution of N independent continuous-time random walks $\eta_1(t)$, $\eta_2(t)$,..., $\eta_N(t)$ on the complete graph on Λ_V, with generators Δ_V, starting from the sites $x_1, x_2,..., x_N \in \Lambda_V$, respectively. Denote by τ the first collision time of these random walks:

$$\tau = \inf\{s \mid \eta_i(s) = \eta_j(s) \text{ for some } i, j \in \{1, 2,..., N\}, i \neq j\}$$

By more or less standard arguments one gets the following representation of the partition function:

$$Z(\beta, N, V) = \frac{1}{N!} \sum_{x_1,..., x_N \in \Lambda_V} \sum_{\pi \in \mathrm{Perm}(N)} \mathscr{P}_{x_1,..., x_N}(\tau > \beta \text{ and } (\forall i)\, \eta_i(\beta) = x_{\pi(i)})$$

Here Perm(N) denotes the group of permutations of N elements. (We do not give here the standard derivation of this formula. One can find very similar derivations in various places in the literature; e.g., refs. 9 and 23.)

Using the fact that any two sets of vertices of the complete graph with the same cardinality are equivalent under the symmetry group of the graph, we easily get from the previous formula

$$Z(\beta, N, V) = \binom{V}{N} \mathscr{P}_{1,\dots,N}(\tau > \beta \text{ and } \{\eta_1(\beta),\dots, \eta_N(\beta)\} = \{1,\dots, N\})$$

(Here $\{\cdots\} = \{\cdots\}$ means equality of the sets.) We want to exploit further the high degree of symmetry of the complete graph. Let us define the following jump process on $\mathbb{Z}_+ \cup \{\dagger\}$:

$$\tilde{Y}^{V,N}(t) = \begin{cases} \frac{1}{2} \# \{1, 2,\dots, N\} \circ \{\eta_1(t), \eta_2(t),\dots, \eta_N(t)\} & \text{for} \quad t < \tau \\ \dagger & \text{for} \quad t \geqslant \tau \end{cases}$$

(The symbol † here has its usual meaning—cemetery; $\circ$ denotes symmetric difference and $\#$ cardinality of finite sets.) $\tilde{Y}^{V,N}(t)$ is a natural measure of the distance between the set of sites occupied by the N random walkers at time t from the starting set; the process $\tilde{Y}^{V,N}$ dies if two random walkers jump on the same site.

Obviously, $\tilde{Y}^{V,N}(t)$ is a continuous-time random walk on $\mathbb{Z}_+ \cup \{\dagger\}$ starting from 0. The dying rate of $\tilde{Y}^{V,N}$ is $N(N-1)/V$, the jump rate is $N(V-N)/V$. The $\tilde{Y}^{V,N}$ can jump by -1, 0, or $+1$ with probabilities

$$\begin{aligned} P^{V,N}_{k\to k+1} &= \frac{(N-k)(V-N-k)}{N(V-N)} \\ &= 1 - \frac{V}{V-N}\frac{k}{N} + \frac{N}{V-N}\left(\frac{k}{N}\right)^2 = r^{V,N}\left(\frac{k}{N}\right) \\ P^{V,N}_{k\to k} &= \frac{k(V-2k)}{N(V-N)} \\ &= \frac{V}{V-N}\frac{k}{N} - \frac{2N}{V-N}\left(\frac{k}{N}\right)^2 = q^{V,N}\left(\frac{k}{N}\right) \qquad (3.1) \\ P^{V,N}_{k\to k-1} &= \frac{k^2}{N(V-N)} \\ &= \frac{N}{V-N}\left(\frac{k}{N}\right)^2 = l^{V,N}\left(\frac{k}{N}\right) \\ & 0 \leqslant k \leqslant \min\{N, V-N\} \end{aligned}$$

The Markov character of the process $\tilde{Y}^{V,N}$ easily follows from the high degree of symmetry (i.e., poor geometry) of the complete graph: the geometric relation of two subsets of cardinality N of Λ_V is completely determined by the degree of overlapping of the two subsets. The calculation of the jump probabilities is straightforward combinatorics.

Thus, we arrive at our final random walk representation of the partition function:

$$\begin{aligned} Z(\beta, N, V) &= \binom{V}{N} \mathscr{P}(\tilde{Y}^{V,N}(\beta) = 0) \\ &= \binom{V}{N} \exp\left(-\frac{N(N-1)}{V}\beta\right) \mathscr{P}(\tilde{Y}^{V,N}(\beta) = 0 \mid \tilde{Y}^{V,N}(\beta) \neq \dagger) \\ &= \binom{V}{N} \exp\left(-\frac{N(N-1)}{V}\beta\right) \mathscr{P}\left(Y^{V,N}\left(\frac{N(V-N)}{V}\beta\right) = 0\right) \end{aligned}$$

In the last line $Y^{V,N}(t)$ is a continuous-time random walk on $\mathbb{Z}_+$ with unit jump rate and jump probabilities given by (3.1), starting from the origin. It is obtained from $\tilde{Y}^{V,N}$ by conditioning to the event that it did not die before time β and a convenient rescale of time.

The existence of the thermodynamic limit (2.1) is equivalent to the existence of the following "rate function":

$$I_\rho(\theta) = -\lim_{\substack{V,N\to\infty \\ N/V\to\rho}} \frac{1}{N} \log \mathscr{P}(Y^{V,N}(N\theta) = 0) \tag{3.2}$$

We will choose $\theta = (1-\rho)\beta$. Using these expressions in (2.1), we get the final formula of this section,

$$\beta f(\rho, \beta) = \rho \log \rho + (1-\rho)\log(1-\rho) + \beta\rho + \rho(I_\rho(\beta(1-\rho)) - \beta(1-\rho)) \tag{3.3}$$

Our problem is now identified as a genuine large-deviation problem related to the family of continuous-time, spatially inhomogeneous random walks $Y^{N,V}(t)$ on $\mathbb{Z}$. As we shall see in the next section, this is exactly the problem of Friedlin and Ventsel' on random perturbations of dynamical systems.[10,19–22] Henceforth we shall concentrate on the calculation of the rate function I_ρ and in the end we shall find it as the solution of a classical variational problem.

4. VENTSEL'S THEOREM

The theory of large deviations of random perturbations of dynamical systems due to Ventsel' and Freidlin is exactly what we need for the study of the limit (3.2). In this order we formulate now as Theorem 2 a very special consequence of Ventsel's Theorem 2.1 in ref. 22, suitable to our problem.

Let

$$l^\varepsilon, r^\varepsilon, l, r\colon \quad \mathbb{R} \to \mathbb{R}_+$$

be uniformly continuous and bounded functions and such that l^ε and r^ε converge uniformly to l and r, respectively, as $\varepsilon \to 0$. Let $Y^\varepsilon(t)$ be the continuous-time Markovian random walk on $\mathbb{Z}$ with jump probabilities given as follows:

$$\mathscr{P}(Y^\varepsilon(t+\Delta t) = x \pm 1 \mid Y^\varepsilon(t) = x) = \begin{cases} r^\varepsilon(\varepsilon x) \cdot \Delta t + o(\Delta t) \\ l^\varepsilon(\varepsilon x) \cdot \Delta t + o(\Delta t) \end{cases}$$

We shall consider the naturally rescaled process

$$\xi^\varepsilon(t) = \varepsilon Y^\varepsilon(t/\varepsilon), \qquad t \in [0, \theta]$$

We denote by $D_0[0, \theta]$ the space of right-continuous trajectories with discontinuities only of the first kind on $[0, \theta]$ starting from the origin, endowed with the Skorohod topology. By $C_0[0, \theta]$ we denote the subspace of continuous trajectories and by $AC_0[0, \theta]$ the subspace of absolutely continuous trajectories. (Note that the Skorohod topology restricted to C_0 is exactly the sup-norm topology. More details about the Skorohod topology can be found in ref. 5.) Clearly, $\xi^\varepsilon \in D_0[0, \theta]$.

It can be shown that the weak law of large numbers holds for the processes ξ^ε, i.e.,

$$\xi^\varepsilon \xrightarrow{\text{Prob}} \bar{y} \qquad \text{in} \quad D_0[0, \theta]$$

where $\bar{y}$ is the unique solution of the ordinary differential equation

$$\dot{\bar{y}} = r(\bar{y}) - l(\bar{y}), \qquad \bar{y}(0) = 0$$

We ask about the large deviations (of order 1) from this LLN trajectory. The answer is given by the following consequence of Ventsel's Theorem 2.1 in ref. 22.

Theorem 2 (A. D. Ventsel'). Under the assumed conditions, the processes $\xi^\varepsilon \in D_0[0, \theta]$ obey the full large-deviation principle governed by the following rate function (or action functional):

$$\mathscr{I}[y] = \begin{cases} \displaystyle\int_0^\theta L(y(s), \dot{y}(s))\, ds + \theta & \\ \qquad \text{if } y \in AC_0[0, \theta] \text{ and the integral is finite} & \\ \infty \qquad \text{otherwise} & \end{cases} \tag{4.1}$$

where the Lagrangian is

$$L(x, v) = \frac{v}{2} \log \left(\frac{[v^2 + 4l(x)\, r(x)]^{1/2} + v}{[v^2 + 4l(x)\, r(x)]^{1/2} - v} \cdot \frac{l(x)}{r(x)} \right) - \{ [v^2 + 4l(x)\, r(x)]^{1/2} + q(x) \} \tag{4.2}$$

and

$$q(x) = 1 - l(x) - r(x)$$

Let us turn back now to our concrete problem. We have the family of continuous-time random walks $Y^{N,V}(t)$ on $\mathbb{Z}$ starting from the origin, with unit jump rate and jump probabilities given in (3.1), and we now ask about the asymptotics of

$$\mathcal{P}\left(Y^{N,V}\left(\frac{N(V-N)}{V-1} \beta \right) = 0 \right)$$

when N, $V \to \infty$ in such a way that $N/V \to \rho$. As this problem is invariant under the change $N \to V - N$, we shall assume from now on that $\rho \leqslant 1/2$ and $N \leqslant V - N$. Thus, the random walks $Y^{N,V}$ are confined to the interval $[0, N]$. The natural setup for our problem is to look at the large deviations of the rescaled processes

$$\xi^{N,V}(t) = \frac{1}{N} Y^{N,V}(Nt), \qquad t \in [0, \theta] \qquad \text{with} \quad \theta = (1-\rho)\beta$$

(As the processes $\xi^{N,V}$ are confined to the interval $[0, 1]$ with probability 1, we need not extend everything to the whole line $\mathbb{R}$.)

In order to apply Theorem 2, we have to identify ε with N^{-1}, and the functions l, r, q: $[0, 1] \to \mathbb{R}_+$ [cf. (3.1)] as follows ($x \in [0, 1]$):

$$\begin{aligned} r(x) &= 1 - \frac{1}{1-\rho} x + \frac{\rho}{1-\rho} x^2 \\ l(x) &= \frac{\rho}{1-\rho} x^2 \\ q(x) &= 1 - l(x) - r(x) = \frac{1}{1-\rho} x - \frac{2\rho}{1-\rho} x^2 \end{aligned} \tag{4.3}$$

When identifying l^ε and r^ε we get exactly the same formulas with N/V instead of ρ; see the right-hand side of (3.1).

The only difference between this setup and Ventsel's original one is that our random walks $Y^{N,V}(t)$ and rescaled processes $\xi^{N,V}(t)$ are confined to the intervals $[0, N]$ and $[0, 1]$, respectively. But, as the conditions of the theorem are satisfied in the interior of these intervals, one can check that all the steps of Ventsel's proof apply.

Thus, the large-deviation principle holds for our rescaled random walk $N^{-1}Y^{N,V}(Nt)$. The rate function $\mathscr{I}_\rho[y]$ is defined in (4.1) with the Lagrangian $L_\rho(x, v)$ defined in (4.2), with the functions l, r, and q given in (4.3).

5. A FIRST LOOK AT THE VARIATIONAL PROBLEM

The expert in large-deviation theory will have guessed already that the limit (3.2) must be determined by the variational expression

$$I_\rho(\theta) = \inf\{\mathscr{I}_\rho[y] \mid y \in C[0, \theta] \text{ such that } y(0) = 0 = y(\theta)\} \tag{5.1}$$

where $\mathscr{I}_\rho$ is defined at the end of the previous section. And indeed, we shall prove this assertion in the next section. But in order to do that, some preparation must be done.

For the moment consider (5.1) as definition of I_ρ. The present section is devoted to the preliminary analysis of this variational problem. To this problem the classical Euler–Lagrange theory applies.[8] As the Euler–Lagrange equation looks rather complicated and we are not going to use it explicitly, we do not write it down here. But according to the Euler–Lagrange theory the following constant of the motion (i.e., "energy") is found:

$$\begin{aligned} v\frac{\partial L_\rho}{\partial v}(x, v) - L_\rho(x, v) &= [v^2 + 4l(x)\, r(x)]^{1/2} + q(x) \\ [\dot{y}(t)^2 + 4l(y(t))\, r(y(t))]^{1/2} &+ q(y(t)) = E \in [0, \infty) \end{aligned} \tag{5.2}$$

where E is constant along trajectories $y(t)$ satisfying the Euler–Langrange equation. Using this conservation law, we find that in the x–v plane the trajectories are the hyperbola branches

$$v^2 = a_E(x - b_E)^2 - c_E, \qquad x \in [0, 1], \qquad v \in \mathbb{R}$$

where

$$\begin{aligned} a_E &= \frac{(1-2\rho)^2 + 4\rho(1-\rho)E}{(1-\rho)^2} \\ b_E &= \frac{(1-\rho)E}{(1-2\rho)^2 + 4\rho(1-\rho)E} \\ c_E &= \frac{4\rho(1-\rho)\, E^2(1-E)}{(1-2\rho)^2 + 4\rho(1-\rho)E} \end{aligned} \tag{5.3}$$

as shown in Fig. 2. [At this point some care is needed, since when rationalizing Eq. (5.2) a family of spurious appears for $E < \max_{0 \leqslant x \leqslant 1} q(x)$.]

In this parametrization, trajectories with $E \in (1, \infty)$ flow from $x = 0$ to $x = 1$ (and back). To $E = 1$ corresponds the LLN trajectory

$$\dot{y} = 1 - \frac{y}{1-\rho}$$

(and the backward motion on the same path). We are interested only in the trajectories in the range of parameters $E \in (0, 1)$ which start from and return to $x = 0$. For E fixed in this range, denote by

$$v_E^{\pm}(x) = \pm[a_E(x-b_E)^2 - c_E]^{1/2}, \qquad x \in [0, \bar{x}_E] \tag{5.4}$$

the velocity as a function of position, where

$$\bar{x}_E = b_E - \left(\frac{c_E}{a_E}\right)^{1/2} = \frac{(1-\rho)E}{1 + [4\rho(1-\rho)(1-E)]^{1/2}} \tag{5.5}$$

is the turning point of this trajectory.

We are ready now to prove the existence of the limit (3.2). After doing that, we shall return to the analysis of the variational problem.

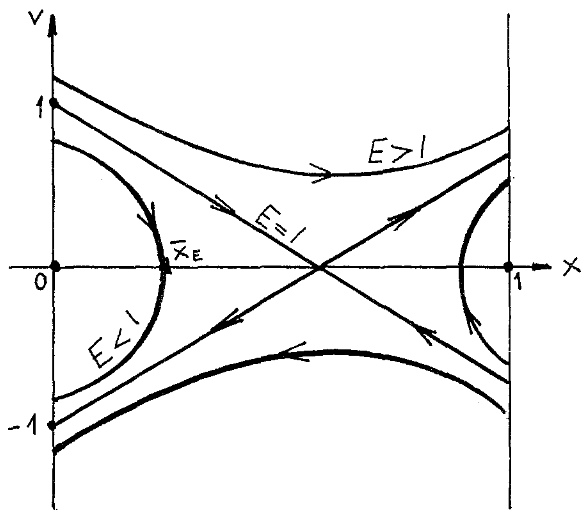

Fig. 2. The flow diagram in the x–v plane.

6. THE EXISTENCE OF THE THERMODYNAMIC LIMIT

In this section we prove the first assertion of Theorem 1. We prove the following.

Lemma 1. The limit (3.2) exists and its value is given by the variational expression (5.1).

The existence of the thermodynamic limit (2.1) follows from this lemma via (3.3).

Proof. The upper bound. As $\{y \in D_0[0, \theta] \mid y(\theta) = 0\}$ is a closed subset of $D_0[0, \theta]$, the upper bound

$$\begin{aligned}
&\limsup_{\substack{N, V \to \infty \\ N/V \to \rho}} \frac{1}{N} \log \mathscr{P}(Y^{N,V}(N\theta) = 0) \\
&\quad = \limsup_{\substack{N, V \to \infty \\ N/V \to \rho}} \frac{1}{N} \log \mathscr{P}(\xi^{N,V}(\theta) = 0) \\
&\quad \leqslant -\inf\{\mathscr{I}_\rho[y] \mid y \in D_0[0, \theta],\ y(\theta) = 0\}
\end{aligned}$$

follows directly from the large-deviation principle of Section 4.

The lower bound. Obviously

$$\begin{aligned}
&\mathscr{P}(Y^{N,V}(N\theta) = 0) \\
&\quad \geqslant \mathscr{P}(Y^{N,V}(N\theta) = 0 \text{ and } Y^{N,V}(N(\theta - \delta)) < N\delta) \\
&\quad \geqslant \mathscr{P}(Y^{N,V}(N(\theta - \delta)) < N\delta) \\
&\qquad \times \min_{0 \leqslant k \leqslant N\delta} \mathscr{P}(Y^{N,V}(N\theta) = 0 \mid Y^{N,V}(N(\theta - \delta)) = k)
\end{aligned} \tag{6.1}$$

As a direct consequence of the large-deviation principle of Section 4 we have

$$\begin{aligned}
&\lim_{\substack{N, V \to \infty \\ N/V \to \rho}} \frac{1}{N} \log \mathscr{P}(Y^{N,V}(N(\theta - \delta)) < N\delta) \\
&\quad = \liminf_{\substack{N, V \to \infty \\ N/V \to \rho}} \frac{1}{N} \log \mathscr{P}(\xi^{N,V}(\theta - \delta) < \delta) \\
&\quad \geqslant -\inf\{\mathscr{I}_\rho[y] \mid y \in D_0[0, \theta],\ y(\theta - \delta) < \delta\}
\end{aligned} \tag{6.2}$$

But from the analysis of the previous section [especially from (5.3) and the flow chart] we see that the trajectory which minimizes (5.1) has speed strictly less than 1, and consequently, for that trajectory, $y(\theta-\delta)<\delta$. Thus, we get

$$\inf\{\mathscr{I}_\rho[y] \mid y\in D_0[0,\theta],\, y(\theta-\delta)<\delta\} \leqslant \inf\{\mathscr{I}_\rho[y] \mid y\in D_0[0,\theta],\, y(\theta)=0\} \tag{6.3}$$

In order to estimate the second factor in the right-hand side of (6.1), observe that for $\forall k\in[0, N\delta]$

$$\begin{aligned}
&\mathscr{P}(Y^{N,V}(N\theta)=0 \mid Y^{N,V}(N(\theta-\delta))=k)\\
&\quad\geqslant e^{-N\delta}\frac{(N\delta)^k}{k!}\prod_{l=1}^{k}\left(\frac{N}{V-N}\frac{l^2}{N^2}\right)\\
&\quad\geqslant e^{-N\delta}\prod_{l=1}^{[N\delta]}\left(\frac{N}{V-N}\frac{l^2}{N^2}\right)
\end{aligned} \tag{6.4}$$

and thus

$$\begin{aligned}
&\liminf_{\substack{N,V\to\infty\\ N/V\to\rho}}\frac{1}{N}\log\big[\min_{0\leqslant k\leqslant N\delta}\mathscr{P}(Y^{N,V}(N\theta)=0 \mid Y^{N,V}(N\theta-\delta))=k)\big]\\
&\quad\geqslant -\delta-\delta\log\frac{1-\rho}{\rho}-2\int_0^\delta \log\left(\frac{1}{s}\right)ds
\end{aligned} \tag{6.5}$$

By combining (6.1)–(6.5) and taking the limits $N\to\infty$, $V\to\infty$, $N/V\to\rho$, and $\delta\to 0$ subsequently, we get the lower bound.

7. EVALUATION OF THE RATE FUNCTION

At the present stage we know that the thermodynamic limit (2.1) exists and the free energy is given by (3.3) with I_ρ defined by the variational expression

$$I_\rho(\theta)=\inf_{y(0)=0=y(\theta)}\int_0^\theta L_\rho(y(s),\dot{y}(s))\,ds+\theta \tag{7.1}$$

The present section is devoted to the evaluation of I_ρ.

We shall do this by fixing a value of the energy $E\in(0,1)$ and calculating θ and I_ρ as functions of this parameter.

Let $y_E(s)$ be the solution of the Euler–Lagrange equation belonging to the energy value E, with initial condition $y_E(0)=0$. We denote by $\hat{\theta}_\rho(E)$ the orbit time and by $\hat{S}_\rho(E)$ the action of this trajectory:

$$\hat{\theta}_\rho(E)=\min\{s>0 \mid y_E(s)=0\}$$

$$\hat{S}_\rho(E)=\int_0^{\hat{\theta}_\rho(E)} L_\rho(y_E(s), \dot{y}_E(s))\, ds$$

Using the explicit form (4.2) of L_ρ and the conservation law (5.2), we express these functions as the following integrals:

$$\hat{\theta}_\rho(E)=2\int_0^{\bar{x}_E} \frac{dx}{v_E^+(x)} \tag{7.2}$$

$$\hat{S}_\rho(E)=\int_0^{\bar{x}_E} \log\frac{E-q(x)+v_E^+(x)}{E-q(x)-v_E^+(x)}\, dx - E\hat{\theta}_\rho(E) \tag{7.3}$$

with $v_E^+(x)$ and $q(x)$ given in (5.4) and (4.3). The integration in (7.2) is straightforward. The orbit time is

$$\hat{\theta}_\rho(E)=\frac{1-\rho}{[(1-2\rho)^2+4\rho(1-\rho)E]^{1/2}}\log\frac{1+[(1-2\rho)^2+4\rho(1-\rho)E]^{1/2}}{1-[(1-2\rho)^2+4\rho(1-\rho)E]^{1/2}}$$

$(0, 1)\ni E\mapsto\hat{\theta}_\rho(E)\in\mathbb{R}_+$ is a C_∞ monotonic increasinig function with

$$\hat{\theta}_\rho(0)=\frac{1-\rho}{1-2\rho}\log\frac{1-\rho}{\rho}=\theta_{\mathrm{cr}}(\rho) \tag{7.4}$$

and

$$\lim_{E\to 1}\hat{\theta}_\rho(E)=\infty$$

Consequently, for any $\theta\in[\theta_{\mathrm{cr}}(\rho), \infty)$ the equation

$$\hat{\theta}_\rho(E)=\theta \tag{7.5}$$

has a unique solution $E(\theta)\in[0, 1)$ and this is a C_∞ function of θ. On the other hand, for $\theta\in[0, \theta_{\mathrm{cr}}(\rho))$, Eq. (7.5) has no solution in $[0, 1)$. This means exactly the following. For $\theta\in(\theta_{\mathrm{cr}}(\rho), \infty)$ the Euler–Lagrange equation with the initial and final condition $y(0)=0=y(\theta)$ has two solutions: (1) $y_0(s)\equiv 0$, $s\in(0, \theta)$ and (2) $y_{E(\theta)}(s)$, $s\in(0, \theta)$. It is easy to see that the second one minimizes (7.1). On the other hand, for $\theta\in[0, \theta_{\mathrm{cr}}(\rho)]$ the only solution of the Euler–Lagrange equation with the given initial and final condition is as (1) above, and consequently this is the minimizer of (7.1).

Thus we have proved the following equality:

$$I_\rho(\theta)-\theta=\begin{cases}0 & \text{if } \theta\in[0, \theta_{\mathrm{cr}}(\rho)]\\ \hat{S}_\rho(E(\theta)) & \text{if } \theta\in(\theta_{\mathrm{cr}}(\rho), \infty)\end{cases} \tag{7.6}$$

The next step is to find a nicer expression for $\hat{S}_\rho(E)$. In this order let us calculate first its derivative with respect to the parameter E:

$$\frac{d\hat{S}_\rho}{dE}(E) = \frac{d\bar{x}_E}{dE} \cdot \log \frac{E - q(\bar{x}_E) + v_E^+(\bar{x}_E)}{E - q(\bar{x}_E) - v_E^+(\bar{x}_E)}$$
$$+ 2\int_0^{\bar{x}_E} \frac{1}{[E - q(x)]^2 - [v_E^+(x)]^2} \left\{ [E - q(x)] \frac{dv_E^+}{dE}(x) - v_E^+(x) \right\} dx$$
$$- \hat{\theta}_\rho(E) - E \frac{d\hat{\theta}_\rho}{dE}(E)$$

But as $v_E^+(\bar{x}_E) = 0$, the first term cancels. Using the conservation law (5.2) and the expression (7.2) for the orbit time, the second and third terms cancel as well and in the end we are left with

$$\frac{d\hat{S}_\rho}{dE}(E) = -E \frac{d\hat{\theta}_\rho}{dE}(E) \tag{7.7}$$

Combining (7.6) and (7.7), we have

$$I_\rho(\theta) - \theta = \begin{cases} 0 & \text{if} \quad \theta \in [0, \theta_{\text{cr}}] \\ -\int_{\theta_{\text{cr}}}^{\theta} E(\theta')\, d\theta' & \text{if} \quad \theta \in (\theta_{\text{cr}}, \infty) \end{cases}$$

After integrating by parts the right-hand side, we get the following.

Lemma 2.

$$I_\rho(\theta) - \theta = \begin{cases} 0 & \text{if } \theta \in [0, \theta_{\text{cr}}] \\ \dfrac{(1-2\rho)^2}{2(1-\rho)\rho}(\theta - \theta_{\text{cr}}) + \dfrac{1}{2\rho}\log[1 - E(\theta)] + \theta E(\theta) & \text{if } \theta \in (\theta_{\text{cr}}, \infty) \end{cases} \tag{7.8}$$

where $E(\theta)$ is the unique solution of (7.5) and $\theta_{\text{cr}} = \theta_{\text{cr}}(\rho)$ is defined in (7.4).

Lemmas 1 and 2 via formula (3.3) give the complete proof of Theorem 1.

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