The "commensurability-non-commensurability" transition in one-dimensional chains

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We consider one-dimensional classical systems with a potential of the $W = \Sigma(V(x_i) + U(x_i + x_{i-1} - \gamma))$ type where V is a periodic potential of period 1 and U is the energy of the interaction between the particles. We show that as $T \to 0$ the limit of the Gibbs distribution is described by an invariant probability distribution for a certain two-dimensional transformation. We study the dependence of such a distribution on the parameter.

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We consider a model of interacting particles placed on a crystalline substrate. We assume that there are only interactions between nearest neighbors and that the interaction is elastic. In the one-dimensional case the potential has then the form

$$U = \sum_i U(x_i - x_{i-1} - \gamma);$$

$$U(-x) = U(x), \quad U(0) = 0, \quad U''(x) \geqslant \text{const} > 0.$$

The parameter γ is equal to the average distance betwen the particles. The effect of the substrate is described by the potential $V(x)$ which is a periodic function having the period of the background, which we take as the unit length. The origin is taken at a point, is assumed to be unique, where V is a minimum. The total potential energy of the system equals

$$W = \sum_i V(x_i) + \sum_i U(x_i - x_{i-1} - \gamma). \tag{1}$$

One-dimensional chains with the interaction (1) have been studied, starting with the work of Frenkel and Kontorova[1] who investigated the case $V(x) = \alpha(1 - \cos 2\pi x)$, $U(x) = x^2$.

Frank and Van der Merwe[2] and Dzyaloshinskiĭ[3] have discussed a continuous variant of such systems. In those papers the possibility of a "commensurability-non-commensurability" type phase transition was first indicated. Recently models of the kind (1) were the subject of active studies in papers by Aubry,[4] Pokrovsky,[5] Bak,[6] and others. We propose in the present paper a new approach to constructing a phase diagram of similar systems at $T = 0$. In the one-dimensional case only such diagrams have a meaning because of the impossibility of phase transitions. We restrict ourselves the range of values $\gamma > 1$. Other regions can be studied in a similar way.

We consider on the segment $[-R, R]$ in the configuration space of the particles a grand canonical Gibbs ensemble with a chemical potential $\mu = 0$. Its density in the subset of N-particle configurations has the form

$$\frac{1}{\Xi} \exp\left\{-\frac{1}{kT}\left[\sum_{i=1}^{N} V(x_i) + \sum_{i=1}^{N-1} U(x_i - x_{i-1} - \gamma)\right]\right\}. \tag{2}$$

Here k is the Boltzmann's constant, T the temperature of the system, and Ξ the grand partition function.

It is convenient in the one-dimensional case to study the Gibbs distribution (2) by using the transfer matrix method (see, e.g., Ref. 7). We put $y_i = \{x_i\}$, where $\{\ldots\}$ is the fractional part sign, and $z_i = x_i - x_{i-1}$. In our problem the transfer matrix describes the transition from (y_{i-1}, z_{i-1}) to (y_i, z_i) and has the form

$$K(y_{i-1}, z_{i-1} | y_i, z_i) = \exp\{-\beta[{}^1/_2 V(y_{i-1}) + {}^1/_2 V(y_i) + U(z_i - \gamma)]\}\delta(y_i - z_i - y_{i-1}), \quad \beta = (kT)^{-1}. \tag{3}$$

The next step consists in normalizing the operator K, using its positive eigenfunction, in order to change to the transfer operator of a Markov chain. To do this we look for positive functions $g_\beta(y)$, $g_\beta^*(y, z)$ for which

$$\lambda_\beta g_\beta(y) = \exp\left\{-\frac{1}{2}\beta V(y)\right\} \int_{-\infty}^{\infty} g_\beta(y + z') \times \exp\left\{-\beta\left[\frac{1}{2} V(y + z') + U(z' - \gamma)\right]\right\} dz', \tag{4}$$

$$\lambda_\beta g_\beta^*(y', z') \exp\{-\beta U(z' - \gamma)\} = \int K(y, z | y' z') g_\beta^*(y, z) \exp[-\beta U(z - \gamma)]\, dy dz. \tag{5}$$

Here the λ_β are the corresponding positive eigenvalues which are the same in (4) and (5).

Using g_β and g_β^* we change to the stochastic kernel

$$Q_\beta(y, z | y', z') = Q_\beta(y | y', z') = \exp\{-\beta[{}^1/_2 V(y) + {}^1/_2 V(y') + U(z' - \gamma)]\} g_\beta(y') (g_\beta(y))^{-1} \lambda_\beta^{-1} \delta(y' - (y + z')). \tag{6}$$

The meaning of this change is that in the thermodynamic limit $R \to \infty$ the Gibbs distribution becomes the probability distribution corresponding to a Markov chain whose states are the pairs (y, z), with y a cyclic variable and z varying from $-\infty$ to $+\infty$, while the transfer operator has the form (6). It is natural to represent the space C of such pairs as a cylinder. The stationary distribution of this Markov chain, which gives the first correlation function of our problem, has the

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density

$$g_\beta(y)\,g_\beta^*(y,\,z)\exp\{-\beta U(z-\gamma)\},$$

where the eigenfunctions g_β and g_β^* are normalized such that

$$\int g_\beta(y)\,g_\beta^*(y,z)\exp\{-\beta U(z-\gamma)\}\,dy\,dz=1.$$

As $\beta\to\infty$ the limit of the Gibbs distribution is concentrated on those configurations for which W takes on a minimum value. Hence we must have $\partial W/\partial x_i=0$ or

$$U'(x_{i+1}-x_i-\gamma)=U'(x_i-x_{i-1}-\gamma)+V'(x_i).$$

We can write this relation in terms of the (y, z) variables in the form

$$U'(z_{i+1}-\gamma)=U'(z_i-\gamma)+V'(y_i),\quad y_{i+1}=y_i+z_i. \tag{7}$$

As U' is a monotonically increasing function, the first equality in (7) allows us to find z_{i+1} uniquely from y_i, z_i.

We introduce the transformation S of the cylinder C, which acts according to the formula

$$S(y,\,z)=(y',\,z'),$$

where

$$U'(z'-\gamma)=U'(z-\gamma)+V'(y),\qquad y'=y+z'(\mathrm{mod}\ 1).$$

In that case (7) means that the configurations where W is a minimum are, indeed, trajectories of the transformation S. In the case of the Frenkel-Kontorova model S transforms into

$$z'=z+2\pi\alpha\sin y,\qquad y'=y+z'.$$

This transformation was studied by Chirikov *et al.* (see the review paper, Ref. 8) in connection with the stochasticity of dynamical systems.

As already mentioned, the first correlation function of our problem is the probability distribution on the cylinder C with a density

$$p_\beta(y,\,z)=g_\beta(y)\,g_\beta^*(y,\,z)\exp\{-\beta U(z-\gamma)\}.$$

In that case

$$P_\beta((y_i,z_i)\in A)=\int_A p_\beta(y,z)\,dy\,dz=P_\beta(A) \tag{8}$$

and is independent of i. Here P_β is the probability evaluated using the Gibbs distribution for our system. Taking the limit as $\beta\to\infty$ we see that the Gibbs distribution as $\beta\to\infty$ turns out to be concentrated on the set of configurations which are trajectories of S while the limit $\lim P_\beta(A)$ as $\beta\to\infty$ is the probability distribution on C and has the property that $P(A)=P(SA)$ since as $\beta\to\infty$ it follows from $(y_i, z_i)\in A$ that $(y_{i+1}, z_{i+1})\in SA$.

The probability distributions satisfying this last relation are called invariant under S (see Ref. 9). We thus find that the limit of the first correlation function as $\beta\to\infty$ is the probability distribution on C invariant under S. It is natural to assume that the phase diagram of our model is a function describing the γ-dependence of P.

There are, in general, many invariant probability distributions for the transformation S. To make clear which of them arises from the Gibbs distribution in the limit as $\beta\to\infty$ we introduce for any probability distribution Q on C the integral

$$h(Q)=\int_C [V(y)+U(z-\gamma)]\,dQ,$$

which has the meaning of the average value of the energy per particle. One can show (see Ref. 10) that for the probability distribution P in which we are interested

$$h(P)=\min h(Q),$$

where the minimum is taken over all invariant probability distributions for S. This last relation is the basic criterion to be used to study the phase diagram. Below we apply this criterion to the case when

$$V(y)=\alpha V_0(y),\qquad U(z)=\tfrac{1}{2}z^2+\alpha U_0(z\alpha^{-1/2}),$$

where

$$U_0(0)=U_0'(0)=U_0''(0)=0,\qquad U_0''(z)\geqslant\mathrm{const}>-1,$$

while α is small. A model with such a potential can naturally be considered to be a small perturbation of the Frenkel-Kontorova model.

We put

$$\gamma=1+\Gamma\alpha^{1/2},\qquad y=Y,\qquad z=1+Z\alpha^{1/2}.$$

We write the transformation S in terms of the variables (Y, Z) in the form

$$\begin{aligned} Z'+U_0'(Z'-\Gamma)&=Z+U_0'(Z-\Gamma)+\alpha^{1/2}V_0'(Y),\\ Y'&=Y+\alpha^{1/2}Z'. \end{aligned} \tag{9}$$

For small α Eq. (9) is the difference approximation with step $\alpha^{1/2}$ for the set of differential equations

$$\frac{dY}{dt}=Z,\qquad \frac{dZ}{dt}=\frac{V_0'(Y)}{1+U_0''(Z-\Gamma)}, \tag{10}$$

as the first of Eqs. (9) can be rewritten up to quantities of order $(Z'-Z)^2$ as follows:

$$Z'-Z=(1+U_0''(Z-\Gamma))^{-1}V_0(Y)\alpha^{1/2}.$$

The set (10) has the first integral

$$\mathscr{H}=-V_0(Y)+Z^2+2ZU_0'(Z-\Gamma)-2U_0(Z-\Gamma),$$

and on the (Y, Z) phase plane its integral curves are the lines of constant $\mathscr{H}$. We consider its structure in more detail. The function

$$G(Z)=Z^2+2ZU_0'(Z-\Gamma)-2U_0(Z-\Gamma)$$

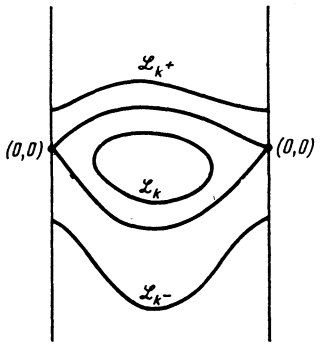

FIG. 1.

is strictly monotonic for $Z \gtrless 0$, as

$$G'(Z)=2Z(1+U_0''(Z-\Gamma))$$

and has the same sign as Z because

$$U_0''(Z-\Gamma) \geqslant \text{const} > -1.$$

Hence, for any k the equation $G(Z)=V_0(Y)+k$ determines two curves $Z=\mathscr{L}_{k\pm}(Y)$. When $k=k_0=G(0)$ these curves go through the point (0,0). When $k<k_0$ these curves are, indeed, the upper and lower parts of a single curve $\mathscr{L}_k$, and when $k>k_0$ the $\mathscr{L}_{k\pm}$ curves are, conversely, different ones. The shape of the $\mathscr{L}_{k\pm}$ is in principle the same as the shape of the integral curves of a physical pendulum, albeit slightly less symmetric (Fig. 1).

As $\alpha \to 0$ the invariant probability distributions of the transformation S go over into the invariant probability distributions for the system (9). For our purposes it is sufficient to restrict ourselves solely to undecomposable, or ergodic, probability distributions which in the case of the system (9) are of three kinds:

1) The probability distribution Q_k concentrated on the curve $\mathscr{L}_k$, $k<k_0$. If we take as the parameter on $\mathscr{L}_k$ the time coordinate, reckoned from some point, we have

$$dQ_k=\Pi_k^{-1}dt,$$

where Π_k is the period of the motion along $\mathscr{L}_k$.

2) The probability distribution $Q_{k\pm}$ concentrated on the curve $\mathscr{L}_{k\pm}$, $k>k_0$. For it also

$$dQ_{k\pm}=\Pi_{k\pm}^{-1}dt.$$

3) The probability distribution $Q^{(0)}$ concentrated on the fixed point (0,0) of the system (9).

The energy integral $h(Q)$ becomes

$$h(Q)=\alpha\int[V_0(Y)+{}^1/_2(Z-\Gamma)^2+U_0(Z-\Gamma)]dQ=\alpha h_0(Q).$$

It is natural to take the phase diagram of the system (9) to mean the function $P(\Gamma)$ with $\Gamma>0$, defined such that for it

$$h_0(P(\Gamma))=\min h_0(Q),$$

where the minimum is taken over the invariant probability distributions for the system (9) of the described three kinds.

We note now that

$$h_0(Q^{(0)})={}^1/_2\Gamma^2-U_0(-\Gamma).$$

It is more convenient to study

$$h_0(Q)-h_0(Q^{(0)})=\int V(Y)\,dQ+\frac{1}{2}\int Z^2dQ-\Gamma\int ZdQ$$
$$+\int(U_0(Z-\Gamma)-U_0(-\Gamma))\,dQ.$$

In the first two cases dQ is proportional to dt and $dt=Z^{-1}dY$. Therefore

$$\int ZdQ=\int dY=0 \quad \text{when } k<k_0,$$
$$\int ZdQ_{k^-}=\int dY=-1 \quad \text{when } k>k_0.$$

If the correction U_0 is sufficiently small, we have

$$h^{(0)}(Q)-h^{(0)}(Q^{(0)})>0$$

for all Q of the form $Q=Q_k$, $k<k_0$ or $Q=Q_{k^-}$, $k>k_0$.

There remain only the probability distributions Q_{k^+}. Here the result now depends on Γ. A more detailed analysis shows the following. We consider the equation for Γ_1:

$$\int_0^1[V_0(Y)-ZU_0(Z-\Gamma_1)+{}^3/_2(U_0(Z-\Gamma_1)$$
$$-U_0(-\Gamma_1))]Z^{-1}dY=\Gamma_1, \qquad (11)$$

where Z is a function of Y by virtue of the equation

$$Z^2+2ZU_0'(Z-\Gamma_1)-2U_0(Z-\Gamma_1)+2U_0(-\Gamma_1)=V_0(Y).$$

Its solution depends, of course, on the form of V_0 and U_0. When $U_0=0$ Eq. (11) can be simplified:

$$\int_0^1[V_0(Y)]^{1/2}dY=\Gamma_1. \qquad (11')$$

The meaning of (11) is that it is equivalent to the relation

$$\left.\frac{dh_0(Q_{k^+})}{dk}\right|_{k=k_0}=0.$$

The phase diagram of the continuous model depends on the solution of Eq. (11). When $\Gamma \leqslant \Gamma_1$ the derivative

$$dh_0(Q_{k^+})/dk>0$$

for all $k>k_0$ and therefore

$$\min_Q h_0(Q)=h_0(Q^{(0)}),$$

i.e., $P=Q^{(0)}$. When $\Gamma>\Gamma_1$ this minimum now depends on Γ. The value $k(\Gamma)$ at which it is reached can be found from the equation

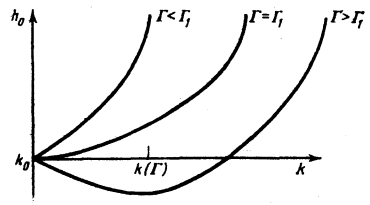

FIG. 2.

$$\frac{d}{dk}h_0(Q_{k^*})=0,$$

which for $U_0=0$ takes the form

$$\int_0^1 [k+V(Y)]^{1/2}\,dY=\Gamma.$$

When $U_0\neq 0$ the form of this equation is very complicated and we do not give it. We show in Fig. 2 the plots of the functions $h_0(Q_{k^*})-h_0(Q^{(0)})$ for different values of Γ.

The reasoning above referred to the continuous limit of our model, which occurs as $\alpha\to 0$. We now consider $\alpha>0$ and study how the phase diagram changes. Initially we consider the structure of the invariant sets of the transformation S.

The point (0,0) is as before a fixed point of S and is of the hyperbolic type. This means that the trajectories of S in the vicinity of (0,0) lie on hyperbola-type curves which are separated by the stable and unstable separatrices $\gamma^{(s)}$ and $\gamma^{(u)}$ (see Fig. 3). When $\alpha=0$ the separatrices $\gamma^{(s)}$ and $\gamma^{(u)}$ coincide in the sense that the continuation of $\gamma^{(s)}$ goes over into $\gamma^{(u)}$, and the other way round. When $\alpha>0$ this is no longer the case and $\gamma^{(s)}$ and $\gamma^{(u)}$ intersect when they are continued, in general at a non-zero angle. The points where the separatrices $\gamma^{(s)}$ and $\gamma^{(u)}$ intersect are called homoclinic points (see Ref. 11). Their intrinsic definition consists in that $S^nA\to(0,0)$ as $n\to\pm\infty$ for any homoclinic point A. Since the angle of intersection of the separatrices is non-zero, a so-called "stochastic layer" (see Ref. 8) is formed in the vicinity of the homoclinic trajectories. The number of different homoclinic trajectories formed is always even and the chaotic behavior manifests itself in the appearance of disordered transitions from one homoclinic trajectory to another.

The width of the stochastic layer is determined by the so-called Mel'nikov-Arnol'd integral (see, e.g., Refs. 12, 13) which in our case has the form

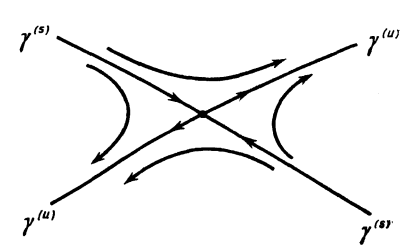

FIG. 3.

$$I=\int_{-\infty}^{\infty}\left[\frac{1}{2}V_0''(Y)Z^2-V_0'(Y)R-R^2(1+ZU_0'''(Z-\Gamma_1)-U_0''(Z-\Gamma_1))\right]dt,$$

$$R(Y,Z)=V_0'(Y)(2(1+U_0''(Z-\Gamma_1)))^{-1}.$$

Here $Y=Y(t)$ and $Z=Z(t)$ are the solution of the set (11) when Γ equals the Γ_1 from (11), for which $Y(t)\to 0$, $t\to-\infty$, and $Y(t)\to 1$ as $t\to\infty$. When $I\neq 0$ the width of the stochastic layer is of order $\alpha^{1/2}$. For the Frenkel-Konotorova model $I=0$ and the width of the stochastic layer is therefore considerably smaller. We shall consider this problem in more detail elsewhere.

We denote the coordinates of the homoclinic points formed when $\gamma^{(s)}$ and $\gamma^{(u)}$ intersect by $(Y^{(i)}, Z^{(i)})$, $i=1, 2, \ldots, 2p$ (see Fig. 4). For the trajectory of each of the homoclinic points $(Y^{(i)}, Z^{(i)})$ we consider its relative energy in relation to the energy of the basic configuration concentrated in (0,0) and for which the points are positioned in the points where the potential V is a minimum. It equals

$$\mathscr{E}^{(i)}=\alpha\sum_{j=-\infty}^{\infty}\left[V_0(Y_j^{(i)})+\frac{1}{2}(Z_j^{(i)})^2+(U_0(Z_j^{(i)})-U_0(-\Gamma))\right],$$

$$(Y_j^{(i)}, Z_j^{(i)})=S^j(Y^{(i)}, Z^{(i)}).$$

We put $\mathscr{E}=\min\mathscr{E}^{(i)}$. It is clear that $\mathscr{E}$ is a function of Γ. We find such $\Gamma_1(\alpha)$ that $\mathscr{E}>0$ for all $0\leqslant\Gamma<\Gamma_1(\alpha)$ and $\mathscr{E}<0$ for $\Gamma>\Gamma_1(\alpha)$. It then turns out (see Ref. 10) that when $I\neq 0$ the point $\Gamma(\alpha)$ possesses the property that when $\Gamma<\Gamma_1(\alpha)$

$$h(Q^{(0)})=\min h(Q).$$

In other words, for such Γ the configuration on which the potential energy reaches a minimum is unique and in that case the points are arranged in the points of the potential minimum. When $\Gamma>\Gamma_1(\alpha)$ this is no longer the case. For arbitrarily small excess above criticality, $\Gamma-\Gamma_1(\alpha)>0$ there are already many such configurations, they lie in the stochastic layer, and the probability distribution P is concentrated in that layer.

Moreover, for small α the Kolmogorov-Arnold-Moser theory (KAM theory) is applicable to the transformation S and it follows from it that the transformation S has many invariant curves close to the curves $\mathscr{L}_k$ and $\mathscr{L}_{k\pm}$ (see Refs. 12, 14). However, these curves do not fill completely the cylinder C and there are also narrow stochastic layers between any two of them. Nonetheless, the area filled by the invariant curves is positive and as $\alpha\to 0$ the fraction of the area occupied by such curves tends to unity.

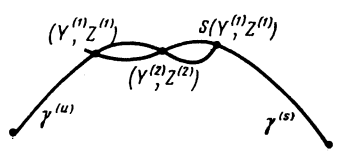

FIG. 4.

We consider the invariant curves close to the curve $\mathscr{L}_{k^+}$. To each such curve we can assign the coordinate r of its point of intersection with the line $Y=0$. In such cases we shall write $\mathscr{L}(r;\alpha)$. The transformation S on the curve $\mathscr{L}(r;\alpha)$ can be reduced to a rotation by means of an appropriate coordinate change. We denote by u the coordinate on $\mathscr{L}(r;\alpha)$ in which S is reduced to a rotation, i.e., $Su=u+\rho$, where $\rho=\rho(r;\alpha)$ is the angle of rotation on $\mathscr{L}(r;\alpha)$. The natural invariant probability distribution $Q(r;\alpha)$ for which $dQ(r;\alpha)=du$ is concentrated on the curve $\mathscr{L}(r;\alpha)$.

There arises the natural problem of how to find for a given α that $\Gamma(r;\alpha)=\Gamma$ for which

$$\min h(Q)=h(Q(r;\alpha)).$$

To simplify some formulae in what follows we consider the case $U_0=0$. We have

$$h(Q(r;\alpha))=\alpha\left[\int V_0(Y)\,du+\int Z^2du-2\Gamma\int Z du+\Gamma^2\right]. \quad (12)$$

The first two integrals are independent of Γ and are functions of r. We consider $\int Z\,du$ in more detail. It is clear that for any point $(Y_0, Z_0)\in\mathscr{L}(r;\alpha)$, $(Y_i, Z_i)=S^i(Y_0, Z_0)$

$$\int Z du=\lim\frac{1}{n}\sum_{i=1}^{n}Z_i.$$

By virtue of (9)

$$\frac{1}{n}\sum_{i=1}^{n}Z_i=\frac{1}{n\alpha^{1/2}}\sum_{i=1}^{n}(Y_{i+1}-Y_i).$$

It is clear from this relation that $\int Z\,du$ characterizes the number of rotations in the coordinate Y, normalized to $\alpha^{-1/2}$, i.e., the average rotation after $\alpha^{-1/2}$ steps. We denote this quantity by $\chi(r;\alpha)$. It is clear that as $\alpha\to 0$ it goes over into the number of rotations for the corresponding curve $\mathscr{L}_{k^+}$.

Differentiating (12) formally with respect to r we find that the value of r for which $h(Q(r;\alpha))$ is a minimum must satisfy the relation

$$\left[2\frac{d\chi(r;\alpha)}{dr}\right]^{-1}\frac{d}{dr}\left[\int_{\mathscr{L}(r;\alpha)}(V_0(Y)+Z^2)\,du=\Gamma.\right.$$

On the other hand, for a given r this equation determines that Γ for which the equation

$$\min h(Q)=h(Q(r;\alpha))$$

is possible. However, as the curves $\mathscr{L}(r;\alpha)$ exist only on the "perforated" set of r values, in principle this last relation is lacking in mathematical precision. This will be seen to elsewhere.

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