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# Can Classical Statistical Mechanics Describe an Infinite Crystal?

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It is shown that $\mathcal{L}^1$-clustering equilibrium states of classical systems of point particles are translationally invariant.

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The search for equilibrium states which are invariant only under some crystallographic subgroup of the full translation group is of considerable interest for the understanding of the solid. In this note we show that such states do not exist under the usual assumptions of statistical mechanics. These assumptions are that infinitely extended states are described by symmetric correlation functions which are $\mathcal{L}^1$ clustering and obey the equilibrium Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy. The class of two-body forces for which the statement holds is very general: The force can have a locally integrable singularity at the origin as well as a long range including the Coulomb case; the result holds also for jellium systems in dimensions $\nu \geqslant 2$.

Precisely, the systems that we consider consist of $N$ species $\alpha = 1, 2, \ldots, N$ of point particles in $\mathrm{R}^\nu$. The particles interact by means of a two-body force which is the sum of a short-range and a long-range part. The short-range part $F_{\alpha_1\alpha_2}(x_1 - x_2)$ is assumed to be antisymmetric, $F_{\alpha_1\alpha_2}(x_1 - x_2) = -F_{\alpha_2\alpha_1}(x_2 - x_1)$ and integrable on $\mathrm{R}^\nu$. The long-range part is of the form $\sigma_{\alpha_1}\sigma_{\alpha_2}F(x_1 - x_2)$, where $\sigma_\alpha$ is the charge of the particle of type $\alpha$, $F(x) = -\nabla\varphi(x)$ is antisymmetric, bounded and has a specific asymptotic behavior. In jellium systems, the rigid homogeneous background of charge density $-\rho_B$ gives rise to the additional one-body force formally given by $-\rho_B\sigma_\alpha\int F(x-y)\,dy$.

We show that in all cases the one-point correlation functions $\rho_\alpha(x)$ are constant. The translational invariance of higher-order correlation functions as well as the details of the proof will be given elsewhere.[1] We treat separately the short-range and the long-range parts of the force. The general situation can be recovered by conjunction of these two cases.

*Short-range force.*—For simplicity, we take only one type of particle. The one-point function $\rho(x_1)$ and the two-point function $\rho(x_1, x_2)$ obey the first two equations of the BBGKY hierarchy (with $T \neq 0$):

$$kT\nabla_{x_1}\rho(x_1) = \int dx_2\, F(x_1 - x_2)\rho(x_1, x_2)\,, \tag{1}$$

$$kT\nabla_{x_1}\rho(x_1, x_2) = F(x_1 - x_2)\rho(x_1, x_2) + \int dx_3\, F(x_1 - x_3)\rho(x_1, x_2, x_3)\,. \tag{2}$$

The following clustering properties are assumed ($\mathcal{L}'$ clustering):

$C_1$: $\rho^T(x_1, x_2) = O(1/|x_1|^{\nu+\epsilon})$ as $|x_1| \to \infty$, $\epsilon > 0$.

$C_2$: $\rho^T(x_1, x_2, x_3) = O(1/|x_1|^{\nu+\epsilon})$ uniformly with respect to $x_2$.

$C_3$: $\int dx_1 \int dx_2\, |\rho^T(x_1, x_2, x_3)| < \infty$.

Here $\rho^T(\cdots)$ are the truncated functions defined in the usual way.

We claim that under the assumptions (1), (2), $C_1$, and $C_2$ or $C_3$, one has $\rho(x)=\rho=\text{const}$ (hereafter referred to as proposition 1). Combining (1) and (2), we find

$$kT\nabla_{x_1}\rho^T(x_1,x_2)=F(x_1-x_2)\rho(x_1,x_2)+\int dx_3\,F(x_1-x_3)[\rho(x_1,x_2,x_3)-\rho(x_1,x_3)\rho(x_2)]. \tag{3}$$

We integrate both sides of Eq. (3) on a sphere $|x_1|\le R$ and let $R\to\infty$. After this integration, the left-hand side of Eq. (3) tends to zero as $R\to\infty$ by $C_1$.

It follows from $C_2$ or $C_3$ that $F(x_1-x_3)[\rho(x_1,x_2,x_3)-\rho(x_1,x_3)\rho(x_2)]$ is an integrable function of $x_1$ and $x_3$ in $\mathbb{R}^\nu\times\mathbb{R}^\nu$ for fixed $x_2$. Therefore, the symmetry of the correlation functions and the antisymmetry of the force implies that the contribution of the last term of Eq. (3) vanishes as $R\to\infty$. We are left with $\int dx_1\,F(x_1-x_2)\rho(x_1,x_2)=0$ which in turn gives $\nabla_{x_1}\rho(x_1)=0$.

One can include stronger singularity of the force at the origin as well as hard cores; this will be discussed at a later date.[2] We should remark that analogous results were discussed previously,[3,4] where it was argued that the onset of long-range order, i.e., $\rho^T(x_1,x_2)$ not integrable, is a necessary condition for the existence of nonuniform liquid-vapor systems.

*Long-range force.*—The asymptotic behavior of $F(x)$ is characterized by

$$F(x)=d(\hat{x})/|x|^\gamma+o(1/|x|^\gamma),\quad \hat{x}=x|x|,\quad d(\hat{x})\ne 0,\quad \nu-1\le\gamma\le\nu;$$

$$(\partial_i F)(x)=O(1/|x|^{\gamma+1}),\quad (\partial_{ij}{}^{(2)}F)(x)=O(1/|x|^{\gamma+2}).$$

We write now the BBGKY equation in the form

$$kT\nabla_{x_1}\rho_{\alpha_1}(x_1)=\sigma_{\alpha_1}E_\rho(x_1)\rho_{\alpha_1}(x_1)+\int dx_2\sum_{\alpha_2}\sigma_{\alpha_1}\sigma_{\alpha_2}F(x_1-x_2)[\rho_{\alpha_1\alpha_2}(x_1,x_2)-\rho_{\alpha_1}(x_1)\rho_{\alpha_2}(x_2)], \tag{4}$$

$$\begin{aligned}kT\nabla_{x_1}\rho_{\alpha_1\alpha_2}(x_1,x_2)&=[\sigma_{\alpha_1}E_\rho(x_1)+\sigma_{\alpha_1}\sigma_{\alpha_2}F(x_1-x_2)]\rho_{\alpha_1\alpha_2}(x_1,x_2)\\&\quad+\int dx_3\sum_{\alpha_3}\sigma_{\alpha_1}\sigma_{\alpha_3}F(x_1-x_3)[\rho_{\alpha_1\alpha_2\alpha_3}(x_1,x_2,x_3)-\rho_{\alpha_3}(x_3)\rho_{\alpha_1\alpha_2}(x_1,x_2)],\end{aligned} \tag{5}$$

where $\rho_{\alpha_1\cdots\alpha_n}(x_1,\ldots,x_n)$ denote the correlation functions and

$$E_\rho(x)=E_0+\int dy[F(x-y)-F(-y)][\textstyle\sum_\alpha\sigma_\alpha\rho_\alpha(y)-\rho_B] \tag{6}$$

$E_\rho(x)$ is the field due to the average charge density and $E_0=E_\rho(x=0)$. In the case $\gamma=\nu-1$ (Coulomb force), we consider only states which are invariant under discrete subgroups of the translations. Such states are necessarily locally neutral.[5] The integral in (6) can then be defined as the limit of definite integrals over any sequence of convex domains converging to $\mathbb{R}^\nu$. Furthermore, one knows that under the clustering assumptions ($C_1$ and $C_2$ or $C_3$) the following sum rule holds true[5]:

$$\sigma_\alpha\rho_\alpha(x)+\int dy\sum_\beta\sigma_\beta\rho_{\alpha\beta}{}^T(x,y)=0. \tag{7}$$

Combining again (4) and (5) as in proposition 1, using Eqs. (6), (7), and the asymptotic properties of the force, one arrives at

$$kT\nabla_x\rho_\alpha(x)=0\quad\text{if}\quad \nu-1<\gamma\le\nu, \tag{8}$$

$$kT\sigma_i\rho_\alpha(x)=-C_\nu\rho_B[x_i\sigma_\alpha\rho_\alpha(x)+\int dy\sum_\beta y_i\sigma_\beta\rho_{\alpha\beta}{}^T(x,y)], \tag{9}$$

with $C_1=2$, $C_2=\pi$, and $C_3=4\pi/3$ in the Coulomb case ($\gamma=\nu-1$). The derivation of (8) is subjected to a slightly stronger condition than $\mathcal{L}'$ clustering, namely that the first moments of the truncated functions are also integrable.

We conclude from (8) that all equilibrium systems with forces decreasing faster than Coulomb are translationally invariant. From Eq. (9), the same result holds for Coulomb systems with $\rho_B=0$. Moreover, for jellium systems ($\rho_B\ne0$), it can be established under the same clustering assumptions that the following additional sum rule has to hold when[6] $\nu\ge2$:

$$x_i\sigma_\alpha\rho_\alpha(x)+\int dy\sum_\beta y_i\sigma_\beta\rho_{\alpha\beta}{}^T(x,y)=0. \tag{10}$$

Therefore, except in one dimension, jellium systems are also translationally invariant. It is known that the one-dimensional jellium is not translationally invariant.[7]

In conclusion if it is possible to describe an infinite crystal within the framework of classical statistical mechanics, then the corresponding states cannot have an integrable clustering.

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# Critical Phenomena on Fractal Lattices

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Renormalization-group techniques are applied to Ising-model spins placed on the sites of several self-similar fractal lattices. The resulting critical properties are shown to vary with the (noninteger) fractal dimensionality $D$, but also with several topological factors: ramification, connectivity, lacunarity, etc. For any $D \geqslant 1$, there exist systems with both $T_c = 0$, and $T_c > 0$; hence a lower critical dimensionality is not defined. The nonvanishing values of $T_c$ and the critical exponents depend on all these factors.

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Noninteger dimensionalities have recently entered physics from at least two separate directions: continuous $\epsilon$ expansions near an integer $d$ in the theory of critical phenomena,[1] and fractals.[2] The $\epsilon$ expansions involve formal analytic continuations of momentum integrals, e.g., $\int d^d q \to \int q^{d-1} dq$,[1] or of recursion relations constructed for $d$-dimensional hypercubic lattices.[3] In these cases, *translational invariance* is assumed (without actual implementation). The resulting general belief is that for systems of given symmetry of the order parameter and interaction range, the critical properties depend *solely* on the dimensionality $d$.[4] In particular, all Ising models with short-range interactions and given $d \geqslant 1$ are believed to exhibit identical critical properties, with the transition temperature $T_c$ decreasing to zero at the lower critical dimensionality $d_l = 1$. Unfortunately, because of the *purely formal* character of the analytic continuations, these beliefs cannot be tested.

By contrast, fractals[2] are *fully explicitly described* geometric shapes, which one may view as "hybrids" between standard (integer $d$) shapes such as lines or planes. A fractal's description involves *several* factors that can vary largely independently of one another: the fractal dimensionality $D$,[5] which is usually not an integer, the topological dimensionality,[6] the order of ramification,[7] the connectivity $Q$,[8] the lacunarity,[9] etc. Note that fractal lattices are scale invariant, but not translationally invariant.

The present Letter reports on the first systematic study of *critical phenomena on fractals*, namely in *spin systems carried by self-similar fractal lattices.*[10] Note that unlike the formal continuations, fractals are themselves *implemented* in real physical systems, e.g., percolation clusters.[2,11] The picture emerging from our application of the renormalization-group techniques to suitably varied fractals is *more complex and subtle* than the present conventional view. *A lower critical dimensionality is not defined.* In fact, the progression between successive integer dimensionalities can be performed in diverse ways, involving very different critical points. As a general rule, Ising systems with given $D$ have $T_c = 0$ if the minimum order or ramification, $R_{\min}$,[7] is finite, and $T_c > 0$ if $R_{\min}$ is infinite.

 