Crystalline Ground States for Classical Particles

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(Received 1 August 2005; published 19 December 2005)

Pair interactions whose Fourier transform is non-negative and vanishes above a wave number K_0 are shown to give rise to periodic and aperiodic infinite volume ground state configurations (GSCs) in any dimension d. A typical three-dimensional example is an interaction of asymptotic form $\cos K_0 r/r^4$. The result is obtained for densities $\rho \geq \rho_d$, where $\rho_1 = K_0/2\pi$, $\rho_2 = (\sqrt{3}/8)(K_0/\pi)^2$, and $\rho_3 = (1/8\sqrt{2}) \times (K_0/\pi)^3$. At ρ_d there is a unique periodic GSC which is the uniform chain, the triangular lattice, and the bcc lattice for $d = 1, 2, 3$, respectively. For $\rho > \rho_d$, the GSC is nonunique and the degeneracy is continuous: *Any* periodic configuration of density ρ with all reciprocal lattice vectors not smaller than K_0, and any union of such configurations, is a GSC. The fcc lattice is a GSC only for $\rho \geq (1/6\sqrt{3}) \times (K_0/\pi)^3$.

DOI: 10.1103/PhysRevLett.95.265501 PACS numbers: 61.50.Ah, 02.30.Nw, 61.50.Lt, 64.70.Dv

Crystallization of fluids is the paradigm of a continuous symmetry breaking. Its conceptual importance has long been recognized [1,2], yet its derivation from first principles is still missing. Nature and computers can easily produce it, but a theoretical understanding of the emergence of a periodic order in continuous space as a result of a translation invariant interaction appears to be particularly hard. The very first step along the way to a proof of a phase transition is to show that such interactions do have periodic ground states. This much more modest program has been advancing also very slowly, and, for a long time, the results were limited mainly to one dimension [3–5]. A ground state configuration (GSC) is a minimizer, in a sense to be defined precisely, of the interaction energy. It is only recently that the mere existence, without characterization, of an infinite volume GSC was proved for a class of interactions in all dimensions [6]. The first two-dimensional example of an interaction giving rise to the triangular lattice as a GSC is even more recent [7]. The main concern of this Letter is to provide examples of ground state ordering in three dimensions. The system we study is composed of identical classical particles interacting via pair interactions whose Fourier transform is non-negative and decays to zero at a $K_0 < \infty$. Our results, although not predictive below a dimension-dependent density $\rho_d \sim K_0^d$, are rather unexpected. At ρ_d a Bravais lattice (bcc for $d = 3$) is the unique periodic GSC. At higher densities, the set of GSC is continuously degenerate: Within certain limits, volume-preserving deformations can be done on every GSC without cost of energy, thus yielding other GSCs. The degeneracy increases with the density, in the sense that compressing any GSC results in a GSC of a higher density that can further be deformed. We can understand this proliferation of GSCs as a consequence of the insensitivity of the interaction to details on a length scale shorter than K_0^{-1}. That bcc lattice can be more stable than fcc should not surprise the reader. At equal densities, the fcc nearest neighbor distance is slightly larger than the bcc one. For a purely repulsive interaction, the fcc lattice is expected to be more stable; for a partly attractive interaction, at some densities the bcc lattice can have a lower energy.

Definitions and notations.—We shall deal with translation invariant symmetric pair interactions $\varphi(\mathbf{r} - \mathbf{r}') = \varphi(\mathbf{r}' - \mathbf{r})$. Rotation invariance will not be supposed. The N-particle configurations ($N \leq \infty$) are subsets of N points of $\mathbb{R}^d$ and will be denoted by Latin capitals B, R, X, Y. Only infinite configurations with a bounded local density will be considered. The number of points in R will be denoted by N_R. If R is a finite configuration, the interaction energy of R is $U(R) = \frac{1}{2}\sum_{\mathbf{r},\mathbf{r}' \in R, \mathbf{r} \neq \mathbf{r}'} \varphi(\mathbf{r} - \mathbf{r}')$. We will assume that φ and $\hat{\varphi}(\mathbf{k}) = \int_{\mathbb{R}^d} \varphi(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r}$ are absolutely integrable on $\mathbb{R}^d$. This ensures that both $\hat{\varphi}$ and $\varphi(\mathbf{r}) = (2\pi)^{-d} \int_{\mathbb{R}^d} \hat{\varphi}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} d\mathbf{k}$ are continuous functions decaying at infinity [8]. In the theorem below, $\hat{\varphi} \geq 0$ implies $U(R) \geq -\varphi(0)N_R/2$, hence, stability [9]. Let R and X be a finite and an infinite configuration, respectively. The energy of R subject to the field created by X is given by

$$U(R|X) = U(R) + \sum_{\mathbf{r} \in R} \sum_{\mathbf{x} \in X} \varphi(\mathbf{r} - \mathbf{x}). \tag{1}$$

Fix a real μ. An infinite configuration X is called a grand canonical ground state configuration for chemical potential μ (μGSC) if it is stable against bounded perturbations; i.e., if for any bounded domain Λ and any R

$$U(R \cap \Lambda | X \setminus \Lambda) - \mu N_{R\cap\Lambda} \geq U(X \cap \Lambda | X \setminus \Lambda) - \mu N_{X\cap\Lambda}, \tag{2}$$

where $X \setminus \Lambda$ is the set of points of X outside Λ. Because every bounded domain is in a parallelepiped, these suffice to be considered. X is a canonical GSC if (2) holds for every R such that $N_{R\cap\Lambda} = N_{X\cap\Lambda}$. Thus, any μGSC is a GSC. If φ is superstable [9], the relation $\mu \mapsto \rho$ (density) is invertible and any GSC is expected to be a μGSC for a suitable μ. Local stability in the sense of Eq. (2) implies global stability; i.e., a GSC minimizes the energy density at the given density; cf. Ref. [10] and the end of this Letter.

A Bravais lattice $B = \{\sum_{\alpha=1}^{d} n_\alpha \mathbf{a}_\alpha | \mathbf{n} \in \mathbb{Z}^d\}$ will be regarded as an infinite configuration. Here $\mathbf{a}_\alpha$ are linearly independent vectors and $\mathbf{n} = (n_1, \ldots, n_d)$ is a d-dimensional integer. Any periodic configuration X can be written as $X = \cup_{j=1}^{J}(B + \mathbf{y}_j)$, where B is some Bravais lattice and $B + \mathbf{y}$ is B shifted by the vector $\mathbf{y}$. For a given X, B is nonunique and we shall choose it so that J is minimum. Then we call X a B-periodic configuration. The reciprocal lattice is $B^* = \{\sum n_\alpha \mathbf{b}_\alpha | \mathbf{n} \in \mathbb{Z}^d\}$, where $\mathbf{a}_\alpha \cdot \mathbf{b}_\beta = 2\pi\delta_{\alpha\beta}$. The nearest neighbor distance (the length of the shortest nonzero vector) in B^* will be denoted by q_{B^*}. This is related to the density via $\rho(B) = c_{\rm type}(q_{B^*})^d$, where $c_{\rm type}$ is determined by the aspect ratios and angles of the primitive cell of B. Let Λ be the parallelepiped spanned by the vectors $L_\alpha \mathbf{a}_\alpha$, $\Lambda = \{\sum x_\alpha \mathbf{a}_\alpha | 0 \le x_\alpha < L_\alpha\}$. We shall take L_α to be positive integers; then Λ is a period cell for B-periodic configurations, and the dual lattice $\Lambda^* = \{\sum (n_\alpha/L_\alpha)\mathbf{b}_\alpha | \mathbf{n} \in \mathbb{Z}^d\}$ contains B^*. Next, we define the *periodized* pair interaction

$$\varphi_\Lambda(\mathbf{r}) = \sum_{\mathbf{n}\in\mathbb{Z}^d} \varphi\left(\mathbf{r} + \sum n_\alpha L_\alpha \mathbf{a}_\alpha\right) \tag{3}$$

and, for R in Λ, the periodized interaction energy $U_\Lambda(R) = \frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'\in R, \mathbf{r}\neq\mathbf{r}'} \varphi_\Lambda(\mathbf{r} - \mathbf{r}')$. The sum defining $\varphi_\Lambda(\mathbf{r})$ is uniformly convergent; therefore, $\varphi_\Lambda(\mathbf{r})$ is continuous and tends to $\varphi(\mathbf{r})$ as each L_α tends to infinity. Finally, let

$$\mu_\Lambda = \mu + \frac{1}{2}\left[\varphi(0) - V(\Lambda)^{-1} \sum_{\mathbf{k}\in\Lambda^*} \hat\varphi(\mathbf{k})\right], \tag{4}$$

where $V(\Lambda)$ is the volume of Λ. μ_Λ tends to μ as Λ increases to $\mathbb{R}^d$.

The main observation leading to the result presented below is as follows. Let $\mathbf{r}_1, \ldots, \mathbf{r}_N$ be any finite configuration. If $\hat\varphi(\mathbf{k}) \ge 0$ and is zero for $|\mathbf{k}| \ge K_0$, then

$$\sum_{i,j=1}^{N} \varphi(\mathbf{r}_i - \mathbf{r}_j) = (2\pi)^{-d} \int_{|\mathbf{k}|<K_0} \hat\varphi(\mathbf{k}) \left| \sum_{j=1}^{N} e^{i\mathbf{k}\cdot\mathbf{r}_j} \right|^2 d\mathbf{k} \ge 0. \tag{5}$$

If we use periodic boundary conditions in a box containing $\mathbf{r}_j$, the integral is to be replaced by a sum. The $\mathbf{k} = \mathbf{0}$ term of this sum is structure-independent (for N fixed) and the rest is non-negative. Hence, any structure making the rest vanish is a GSC. But that is exactly what periodic structures accomplish, provided their shortest reciprocal lattice vector is outside the $|\mathbf{k}| = K_0$ sphere.

THEOREM. Let both φ and $\hat\varphi$ be absolutely integrable in $\mathbb{R}^d$, $\hat\varphi(\mathbf{k}) = \hat\varphi(-\mathbf{k}) \ge 0$ and $\hat\varphi(\mathbf{k}) = 0$ for $|\mathbf{k}| \ge K_0$. We have the following results.

(i) Let B be a Bravais lattice with $q_{B^*} \ge K_0$. Then every B-periodic configuration X is a GSC, and its energy per volume $e(X) = \frac{1}{2}\rho[\rho\hat\varphi(0) - \varphi(0)]$ is minimum for the density $\rho = \rho(X)$. On every period cell Λ, $X \cap \Lambda$ minimizes $U_\Lambda(R)$ for fixed $N_R = N_{X\cap\Lambda}$. Also, X creates a force-free field on test particles; i.e., $U(\mathbf{r}|X)$ is independent of $\mathbf{r}$. Any union of GSCs of the above type is a GSC (that can be aperiodic).

(ii) There is a smallest density ρ_d at which $q_{B^*} = K_0$ holds for a single Bravais lattice. If $\hat\varphi(\mathbf{k}) > 0$ for $0 < |\mathbf{k}| < K_0$, this B is the only periodic GSC. $\rho_1 = K_0/2\pi$, $\rho_2 = (\sqrt{3}/8)(K_0/\pi)^2$, and $\rho_3 = (1/8\sqrt{2})(K_0/\pi)^3$, and the respective GSCs are the uniform chain, the triangular lattice, and the bcc lattice. The fcc, simple hexagonal (sh), simple cubic (sc), and hcp lattices are GSCs at and above the respective densities $\rho_{\rm fcc} = (1/6\sqrt{3})(K_0/\pi)^3$, $\rho_{\rm sh} = (\sqrt{3}/16)(K_0/\pi)^3$, $\rho_{\rm sc} = (1/8)(K_0/\pi)^3$, and $\rho_{\rm hcp} = (4/3\sqrt{3})(K_0/\pi)^3$.

(iii) Suppose, in addition, that $\hat\varphi(0) > 0$ and $[\mu + \frac{1}{2}\varphi(0)]/\hat\varphi(0) \ge \rho_d$. Then any B-periodic configuration X such that $q_{B^*} \ge K_0$ [equivalently, $\rho(B) \ge \rho_d$] and $\rho(X) = [\mu + \frac{1}{2}\varphi(0)]/\hat\varphi(0)$ is a μGSC, and its energy density $e_\mu(X) = e(X) - \mu\rho(X) = -\frac{1}{2}\rho(X)^2\hat\varphi(0)$ is minimum for the given μ. If Λ is a period cell, $X \cap \Lambda$ minimizes $U_\Lambda(R) - \mu_\Lambda N_R$.

Because all the moments of $\hat\varphi$ are finite, φ is infinitely differentiable. A hard-core interaction can be added to φ, provided that the close-packing density is larger than ρ_d. Its only role is to restrict the set of allowed configurations. The set of GSCs is reminiscent of a compressible fluid. The canonical and grand canonical ground state energy densities,

$$e_\rho = \frac{\rho}{2}[\rho\hat\varphi(0) - \varphi(0)], \quad e_\mu = -\frac{1}{2\hat\varphi(0)}\left[\mu + \frac{\varphi(0)}{2}\right]^2, \tag{6}$$

are Legendre transforms of each other,

$$e_\rho = \max_\mu\{e_\mu + \mu\rho\}, \qquad e_\mu = \min_\rho\{e_\rho - \mu\rho\}. \tag{7}$$

The ρ dependence of e_ρ shows that the interaction is stable if $\hat\varphi(0) \ge 0$ and is superstable [9] if $\hat\varphi(0) > 0$. In the second case, (7) expresses the equivalence of the canonical and grand canonical ensembles. The corresponding density and chemical potential satisfy the equation

$$\mu + \varphi(0)/2 - \hat\varphi(0)\rho = 0. \tag{8}$$

This linear relation breaks down for small densities, because μ has to tend to $-\infty$ as ρ approaches zero. This implies a nonanalyticity, presumably at ρ_d.

Examples.—Based on a result on Fourier transforms [11], we can obtain fast-decaying (but not finite-range) interactions satisfying the conditions of the theorem. Take any locally integrable real function $g(\mathbf{k}) = g(-\mathbf{k}) \ge 0$, fix an $\varepsilon > 0$, and define $\hat\varphi(\mathbf{k}) = \int_{|\mathbf{k}'|<K_0-\varepsilon} g(\mathbf{k}')\eta_\varepsilon(\mathbf{k} - \mathbf{k}')d\mathbf{k}'$, where $\eta_\varepsilon(\mathbf{k}) = \exp[-(1 - k^2/\varepsilon^2)^{-1}]$ if $k < \varepsilon$ and 0 otherwise. This $\hat\varphi$ is infinitely differentiable. By inverse-Fourier transforming it, we find φ to decay faster than algebraically. More interesting are the long-range interactions. They can be obtained by choosing $\hat\varphi$ to be only finitely many times differentiable (namely, at $|\mathbf{k}| = K_0$).

For example, in one dimension $\hat{\varphi}(k) = K_0 - |k|$ for $|k| \leq K_0$ yields $\varphi(x) = (1 - \cos K_0 x)/\pi x^2$. In three dimensions, rotation invariant examples can be obtained by starting with a function $f(k) \geq 0$ such that f is 3 times continuously differentiable and $f(K_0) = f'(K_0) = 0$. Then, defining $\hat{\varphi}(\mathbf{k}) = f(|\mathbf{k}|)$ for $|\mathbf{k}| \leq K_0$, by partial integration

$$\varphi(\mathbf{r}) = \frac{1}{2\pi^2 r^4}\left\{[(kf)'' \cos kr]_0^{K_0} - \int_0^{K_0} (kf)''' \cos kr dk\right\}. \tag{9}$$

For instance, $f(k) = \pi^2(k + z)(k + \bar{z})(k - K_0)^2$ with $z = (K_0/10)(1 + 3i)$ gives $\varphi(\mathbf{r}) = (13/10)K_0^3 \cos K_0 r/r^4 + O(1/r^5)$. The higher order terms make φ finite at the origin. One can verify that $\varphi(0)/2\hat{\varphi}(0) > \rho_3$, so this interaction has a continuous family of inequivalent μGSC at $\mu = 0$. Also, it has the bcc lattice as the unique periodic GSC at density $(1/8\sqrt{2})(K_0/\pi)^3$.

LEMMA. Let Λ be a parallelepiped spanned by the vectors $L_\alpha \mathbf{a}_\alpha$. Then

$$\varphi_\Lambda(\mathbf{r}) = V(\Lambda)^{-1} \sum_{\mathbf{k}\in\Lambda^*} \hat{\varphi}(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{10}$$

In one dimension, for $r = 0$, Eq. (10) reduces to the Poisson summation formula [8].

Proof of the lemma.—The Fourier coefficients of φ_Λ are $\int_\Lambda \varphi_\Lambda(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} d\mathbf{r}$. Substituting the sum (3) for $\varphi_\Lambda(\mathbf{r})$, integrating by terms, and resumming, we obtain $\hat{\varphi}(\mathbf{k})$. The series on the right is a continuous periodic function whose Fourier coefficients are also $\hat{\varphi}(\mathbf{k})$. Because of the completeness of the system $\{e^{i\mathbf{k}\cdot\mathbf{r}} | \mathbf{k} \in \Lambda^*\}$ in the Banach space of integrable functions on Λ, equality for all $\mathbf{r}$ follows.

Proof of the theorem.—(i), (iii) Consider the periodic configuration $X = \cup_{j=1}^J (B + \mathbf{y}_j)$ and let R be obtained from X by a bounded perturbation. Take a period parallelepiped Λ of X large enough to contain the perturbed part, that is, $R = X$ outside Λ. Recall that Λ^* contains B^* as a part. For a $\mathbf{k}$ in Λ^*,

$$\sum_{\mathbf{x}\in X\cap\Lambda} e^{-i\mathbf{k}\cdot\mathbf{x}} = \chi_{B^*}(\mathbf{k}) N_{B\cap\Lambda} \sum_{j=1}^J e^{-i\mathbf{k}\cdot\mathbf{y}_j}, \tag{11}$$

where $\chi_{B^*}(\mathbf{k}) = 1$ if $\mathbf{k}$ is in B^* and 0 otherwise. Using the lemma and Eq. (11), after some computation, one finds

$$U(R\cap\Lambda | X\setminus\Lambda) = -\frac{1}{2}\varphi(0) N_{R\cap\Lambda} + \int \frac{\hat{\varphi}(\mathbf{k})}{2(2\pi)^d}\left[\left|\sum_{\mathbf{r}\in R\cap\Lambda} e^{i\mathbf{k}\cdot\mathbf{r}}\right|^2 - 2\sum_{\mathbf{r}\in R\cap\Lambda} e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{x}\in X\cap\Lambda} e^{-i\mathbf{k}\cdot\mathbf{x}}\right] d\mathbf{k} + \rho(B)\sum_{\mathbf{k}\in B^*}\hat{\varphi}(\mathbf{k})\sum_{j=1}^J e^{-i\mathbf{k}\cdot\mathbf{y}_j}\sum_{\mathbf{r}\in R\cap\Lambda} e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{12}$$

Here $\rho(B) = N_{B\cap\Lambda}/V(\Lambda)$, the density of B. We can obtain $U(X\cap\Lambda | X\setminus\Lambda)$ from Eq. (12) if we replace R by X and reapply Eq. (11). Finally, the condition (2) reads

$$\frac{1}{2}(2\pi)^{-d}\int \hat{\varphi}(\mathbf{k})\left|\sum_{\mathbf{x}\in X\cap\Lambda} e^{i\mathbf{k}\cdot\mathbf{x}} - \sum_{\mathbf{r}\in R\cap\Lambda} e^{i\mathbf{k}\cdot\mathbf{r}}\right|^2 d\mathbf{k} \geq (N_{R\cap\Lambda} - N_{X\cap\Lambda})[\mu + \varphi(0)/2 - \rho(X)\hat{\varphi}(0)] + \rho(B)\sum_{0\neq\mathbf{k}\in B^*}\hat{\varphi}(\mathbf{k})\left[N_{B\cap\Lambda}\left|\sum_{j=1}^J e^{i\mathbf{k}\cdot\mathbf{y}_j}\right|^2 - \sum_{j=1}^J e^{-i\mathbf{k}\cdot\mathbf{y}_j}\sum_{\mathbf{r}\in R\cap\Lambda} e^{i\mathbf{k}\cdot\mathbf{r}}\right]. \tag{13}$$

Here we used $N_{X\cap\Lambda} = JN_{B\cap\Lambda}$, $\rho(X) = J\rho(B)$. If $\hat{\varphi}(\mathbf{k}) \geq 0$ and is zero for $|\mathbf{k}| \geq q_{B^*}$, the left member is non-negative, and the sum multiplying $\rho(B)$ vanishes for all R. These and $N_{R\cap\Lambda} = N_{X\cap\Lambda}$ ensure that (13) holds true, so that X is a GSC. If, moreover, $\rho(X) = [\mu + \varphi(0)/2]/\hat{\varphi}(0)$, the first term of the right member also vanishes for all R, and X is a μGSC.

Choosing any period parallelepiped Λ, the canonical energy density of a B-periodic X of density ρ is

$$\begin{aligned} e(X) &= \frac{1}{2V(\Lambda)}\sum_{\mathbf{x}\in X\cap\Lambda}\sum_{\mathbf{x}\neq\mathbf{x}'\in X}\varphi(\mathbf{x}-\mathbf{x}') \\ &= \frac{1}{2V(\Lambda)}\sum_{\mathbf{x},\mathbf{x}'\in X\cap\Lambda}\varphi_\Lambda(\mathbf{x}-\mathbf{x}') - \frac{1}{2}\varphi(0)\rho \\ &= \frac{1}{2}\rho(B)^2\sum_{\mathbf{k}\in B^*}\hat{\varphi}(\mathbf{k})\left|\sum_{j=1}^J e^{i\mathbf{k}\cdot\mathbf{y}_j}\right|^2 - \frac{1}{2}\varphi(0)\rho. \end{aligned} \tag{14}$$

If $\hat{\varphi}(\mathbf{k}) = 0$ for $|\mathbf{k}| \geq q_{B^*}$, then $e(X) = \frac{1}{2}\hat{\varphi}(0)\rho^2 - \frac{1}{2}\varphi(0)\rho$. If also $\hat{\varphi} \geq 0$, then X is a GSC and $e(X)$ is the absolute minimum among configurations of density ρ.

For R in Λ and using again the lemma,

$$U_\Lambda(R) = \frac{1}{2V(\Lambda)}\sum_{0\neq\mathbf{k}\in\Lambda^*}\hat{\varphi}(\mathbf{k})\left|\sum_{\mathbf{r}\in R} e^{i\mathbf{k}\cdot\mathbf{r}}\right|^2 + \frac{N_R}{2V(\Lambda)} \times \left[N_R\hat{\varphi}(0) - \sum_{\mathbf{k}\in\Lambda^*}\hat{\varphi}(\mathbf{k})\right], \tag{15}$$

cf. Eq. (5). If $R = X\cap\Lambda$, according to (11), the first sum reduces to $\mathbf{0} \neq \mathbf{k} \in B^*$ and vanishes completely if $\hat{\varphi}(\mathbf{k}) = 0$ at $|\mathbf{k}| \geq q_{B^*}$. When $\hat{\varphi} \geq 0$, $X\cap\Lambda$ minimizes $U_\Lambda(R)$ for fixed $N_R = N_{X\cap\Lambda}$ and $U_\Lambda(R) - \mu_\Lambda N_R$ under the stronger conditions of (iii). One can also show the opposite implication: If X is periodic and $X\cap\Lambda_n$ minimizes U_{Λ_n} for a sequence $\Lambda_n \to \mathbb{R}^d$ of period cells, then X is a GSC.

With Λ the primitive unit cell,

$$U(\mathbf{r}|X) = \sum_{\mathbf{x}\in X}\varphi(\mathbf{r}-\mathbf{x}) = \sum_{\mathbf{x}\in X\cap\Lambda}\varphi_\Lambda(\mathbf{r}-\mathbf{x}) = V(\Lambda)^{-1}\sum_{\mathbf{x}\in X\cap\Lambda}\sum_{\mathbf{k}\in B^*}\hat{\varphi}(\mathbf{k})e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{x})} = \rho(X)\hat{\varphi}(0), \quad (16)$$

independent of $\mathbf{r}$. This implies that the union of GSCs is also a GSC that can be aperiodic; see [12] for details.

(ii) The one-dimensional case is obvious. In two dimensions, $\rho(B) = (2\pi)^{-2}|\mathbf{b}_1 \times \mathbf{b}_2|$; in three dimensions, $\rho(B) = (2\pi)^{-3}|(\mathbf{b}_1 \times \mathbf{b}_2)\cdot\mathbf{b}_3|$. We are going to select B^* by choosing $\mathbf{b}_\alpha$ in such a way that $\rho(B)$ is minimum, on the condition that $q_{B^*} \equiv \min_{\mathbf{n}\neq\mathbf{0}}\{|\sum n_\alpha \mathbf{b}_\alpha|\} = K_0$. The resulting Bravais lattice at the given density will be denoted by B_d. In two dimensions, let $\mathbf{b}_1$ be one of the shortest vectors of B^*, so that $b_1 = q_{B^*}$. Consider the shortest vectors of B^* not collinear with $\mathbf{b}_1$. These form a star: With $\mathbf{k}$, $-\mathbf{k}$ is also in the set. Choose $\mathbf{b}_2$ among them so that $\mathbf{b}_1\cdot\mathbf{b}_2 \geq 0$. In the triangle of sides b_1, b_2, and $|\mathbf{b}_2 - \mathbf{b}_1|$, we have $|\mathbf{b}_2 - \mathbf{b}_1| \geq b_2 \geq b_1$, so the largest angle is that of the vectors $\mathbf{b}_1$ and $\mathbf{b}_2$. Therefore, this angle α_{12} is between $\pi/3$ and $\pi/2$. Under these restrictions, the minimum of $|\mathbf{b}_1 \times \mathbf{b}_2|$ is obtained for $b_2 = b_1$ and $\alpha_{12} = \pi/3$. These conditions define a triangular lattice for B_2^* and also a triangular lattice for B_2, so that $\rho_2 = \rho_{\mathrm{tr}}$. In three dimensions, the threshold densities of cubic lattices, at which the length of their shortest reciprocal lattice vector is K_0, can simply be computed. This gives the order $\rho_{\mathrm{bcc}} < \rho_{\mathrm{fcc}} < \rho_{\mathrm{sc}}$ and the values presented in the theorem. For the hexagonal lattice, the threshold density depends on c/a, and the minimum is obtained for $c/a = \sqrt{3}/2$. Its value and that of the hcp lattice at $c/a = \sqrt{8}/3$ and $J = 2$ are given in the theorem. It remains to convince oneself that the other Bravais lattices cannot give a smaller density. After some reflection, one can conclude that the conditional minimum of $|(\mathbf{b}_1 \times \mathbf{b}_2)\cdot\mathbf{b}_3|$ is attained by choosing $b_1 = b_2 = b_3 = K_0$ and $\pi/3$ for the three angles between the three pairs of vectors. This specifies B_3^* as an fcc lattice and B_3 as a bcc lattice. Thus, $\rho_3 = \rho_{\mathrm{bcc}}$. The last step of the proof of the theorem is to show that, at the density ρ_d, no other periodic configuration X can be a GSC. Suppose, therefore, that $\rho(X) = \rho_d$. If X is B-periodic but $X \neq B$, then $\rho(B) = \rho_d/J < \rho_d$ and, therefore, $q_{B^*} < K_0$. If $X = B$ but $B \neq B_d$, then again $q_{B^*} < K_0$. Because $\hat{\varphi}(\mathbf{k}) > 0$ for $|\mathbf{k}| < K_0$, at least two nonzero vectors of B^* give a positive contribution to the energy density (14). Hence, $e(X) > \frac{1}{2}\rho_d[\rho_d\hat{\varphi}(0) - \varphi(0)] = e(B_d)$ while $\rho(X) = \rho(B_d)$. Then X is not a GSC because of the following.

Let X and Y be two configurations of equal densities, but let $e(Y) < e(X)$. Then X cannot be a GSC of φ. In other words, every GSC minimizes the energy density at the given number density. Thus, no GSC can be metastable; cf. Ref. [10]. We only outline the proof; details will be given elsewhere [12]. Take a large domain Λ of volume V such that $N_{X\cap\Lambda} = N_{Y\cap\Lambda}$. Estimate

$$U(X\cap\Lambda|X\setminus\Lambda) = U(X\cap\Lambda) + \sum_{\mathbf{x}\in X\cap\Lambda}\sum_{\mathbf{x}'\in X\setminus\Lambda}\varphi(\mathbf{x}-\mathbf{x}').$$

The first term is $V(\Lambda)e(X) + o(V)$, while the second is $o(V)$. Similarly, $U(Y\cap\Lambda|X\setminus\Lambda) = V(\Lambda)e(Y) + o(V)$. Thus, $U(Y\cap\Lambda|X\setminus\Lambda) < U(X\cap\Lambda|X\setminus\Lambda)$ for Λ large enough. This concludes the proof of the theorem.

In summary, for a class of translation invariant pair interactions, we have proved the existence of periodic and aperiodic ground states in classical particle systems. This result is probably the first of its kind in three dimensions. Our finding that ground states of innocent looking RKKY-type interactions such as $\cos K_0 r/r^4$ are continuously deformable by volume-preserving transformations without cost of energy is quite unexpected. In another interpretation, this means that existing crystal structures are stable against perturbations with interactions described in this Letter.

I thank G. Oszlányi, C. Pfister, C. Radin, G. Sewell, J. Sólyom, and F. Theil for helpful remarks. This work was supported by OTKA Grants No. T 042914 and No. T 043494.

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