From bcc to fcc: Interplay between oscillating long-range and repulsive short-range forces

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This paper supplements and partly extends an earlier presentation [Phys. Rev. Lett. **95**, 265501 (2005)]. In d-dimensional continuous space we describe the infinite volume ground state configurations (GSCs) of pair interactions φ and $\varphi+\psi$, where φ is the inverse Fourier transform of a non-negative function vanishing outside the sphere of radius K_0, and ψ is any non-negative finite-range interaction of range $r_0 \leq \gamma_d/K_0$, where $\gamma_3=\sqrt{6}\pi$. In three dimensions the decay of φ can be as slow as $\sim r^{-2}$, and an interaction of asymptotic form $\sim\cos(K_0 r+\pi/2)/r^3$ is among the examples. At a dimension-dependent density ρ_d the ground state of φ is a unique Bravais lattice, and for higher densities it is continuously degenerate: any union of Bravais lattices whose reciprocal lattice vectors are not shorter than K_0 is a GSC. Adding ψ decreases the ground state degeneracy which, nonetheless, remains continuous in the open interval (ρ_d,ρ_d'), where ρ_d' is the close-packing density of hard balls of diameter r_0. The ground state is unique at both ends of the interval. In three dimensions this unique GSC is the bcc lattice at ρ_3 and the fcc lattice at $\rho_3'=\sqrt{2}/r_0^3$.

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I. INTRODUCTION

In an earlier paper[1] we described the infinite volume ground state configurations (GSCs) of a class of classical particle interactions in $d \geq 1$ dimensional continuous space. These pair interactions have a non-negative Fourier transform vanishing above some finite wave number, K_0. We proved that at a threshold density $\rho_d \propto K_0^d$ there is a unique periodic GSC (the basic-centered cubic lattice in three dimensions), and above ρ_d the set of GSCs is continuously degenerate and contains periodic and aperiodic configurations. While this was probably the first result providing specific examples in three (and higher) dimensions, important rigorous work preceded it in lower dimensions; see, for instance, Kunz[2] on the one-dimensional one-component plasma, Ventevogel, Nijboer, and Ruijgrok[3] and Radin[4] on ground states in one dimension and Theil's recent proof of ground state crystallization in two dimensions.[5] Although we will be concerned only with ground state ordering, let us note that rigorous results on phase transitions or ordering in a continuum at positive temperatures do not abound, and all are about more or less contrived model systems. The one-component plasma in one dimension is ordered at all temperatures;[2] Ruelle[6] proved segregation in a two-component system (the Widom-Rowlinson model); Lebowitz, Mazel, and Presutti[7] proved vapor-liquid transition for particles with two-body attractive and four-body repulsive interactions near the mean-field limit; in a one-dimensional model with an unstable interaction low-temperature freezing into an ordered configuration was shown by the present author;[8] and recently Bowen *et al.* proved fluid-solid phase transition in a two-dimensional system of decorated hard hexagons.[9]

In this paper we supplement and partly extend the results of Ref. 1. Apart from recalling the definitions, we do not repeat what is written there. The main part of the theorem of Ref. 1 will be stated and proven in a simpler form, emphasizing the nice algebraic structure of the set of GSCs. Moreover, the results will be extended to interactions of a nonintegrable decay. The proof in Ref. 1 was based on the Poisson summation formula. This formula is widely used in physics; one of its earliest and most famous applications was the calculation of the Madelung constant of ionic crystals by Ewald.[10] The formula involves at least one infinite summation, and neither the convergence of the infinite sum(s) nor the equality of the two sides is guaranteed. Although the results of Ref. 1 were already formally valid to the larger class of interactions, we stated them only for a restricted class, those of the strongly tempered interactions (see later), because no argument supporting the applicability of the Poisson formula to functions of a nonintegrable decay was given in that paper. The extension of this formula constitutes an active field of research in mathematics, see e.g., Ref. 12, but is not our main concern here. Therefore, without looking for the most general formulation, we propose an extension just suitable for our purposes. As a matter of fact, the extension involves also the notion of a ground state configuration. The definition of a GSC is based on infinite sums that are absolutely convergent for strongly tempered interactions, but only conditionally convergent for interactions of a nonintegrable decay, and the way they converge must be specified.

Another, gratuitous, extension, mentioned but not exploited in Ref. 1, will be obtained by modifying the short-range behavior of the interaction. The inverse Fourier transform φ of an integrable function is bounded and continuous—this is our case. Such bounded functions play a role as soft effective interactions in polymer physics,[13] but not in traditional solid state physics where Pauli exclusion gives rise to a practically infinite repulsion at overlaps of atoms. Imagine, however, that an infinite configuration X was shown to be a GSC of φ. Then X will be a GSC of all interactions $\varphi+\psi$, where ψ is non-negative and vanishes at and above the nearest-neighbor distance of X: ψ does not contribute to the specific energy of X, and can only increase the energy of any perturbation of X. Reversing the argument, we may start with $\varphi+\psi$, where ψ is of bounded support, non-negative and may contain a hard core or diverge at the origin as fast as we wish. Then $\varphi+\psi$ has common GSCs with

φ if the support of ψ is small enough and the density is not too high.

The physical importance of the above two extensions is that with them we obtain the GSCs of interactions whose asymptotic form is $\sim\cos K_0 r/r^3$, as that of the RKKY interaction, but which can be arbitrarily strongly repulsive at small distances. As noted also by Likos,[14] such interactions can model those between ions in metals and be relevant in the explanation of the crystal structure of certain metals. However, further study is necessary before any conclusion could be drawn about this question. As an immediate gain, we will find that at some density $\rho_3' > \rho_3$ the unique GSC of $\varphi+\psi$ is the fcc lattice, while at ρ_3 it is the bcc lattice. This transition from bcc to fcc with an increasing density is the consequence of an interplay between a long-range oscillating interaction (which is short range in Fourier space) and a short-range positive pair potential.

The following section is the central part of the paper. After introducing the necessary definitions we announce a theorem in a rather compact form, and then expand its content in a series of remarks. The Poisson summation formula is presented here as a lemma. In Sec. III we prove the lemma, an auxiliary statement about Bravais lattices, and the theorem. This section also contains the proof of a general assertion about the nonexistence of metastable ground states. The paper is closed with a brief summary.

II. DEFINITIONS, NOTATIONS, RESULTS

We consider a system of identical classical particles in $\mathbb{R}^d$, that interact through translation invariant symmetric pair interactions, $\varphi(\mathbf{r}-\mathbf{r}')=\varphi(\mathbf{r}'-\mathbf{r})$. Rotation invariance is not supposed. An N-particle configuration ($N\leq\infty$) is a sequence $(\mathbf{r}_1,\ldots,\mathbf{r}_N)$ of N points of $\mathbb{R}^d$ and will be denoted by B (referring always to a Bravais lattice), R, X, and Y. While the order of the points is unimportant, two or more particles may coincide in a point, resulting $\mathbf{r}_{i_1}=\cdots=\mathbf{r}_{i_m}$. Such a coincidence can occur if $\varphi(\mathbf{0})$ is finite, and it indeed occurs in certain GSCs to be described below. Throughout the paper, the notation φ will be reserved to bounded interactions; unbounded interactions, such as those diverging at the origin or including a hard core, will be composed as $\varphi+\psi$. The number of points in R will be denoted by N_R. The energy of a finite configuration R is

$$U(R)=\frac{1}{2}\sum_{\mathbf{r},\mathbf{r}'\in R,\mathbf{r}\neq\mathbf{r}'}\varphi(\mathbf{r}-\mathbf{r}'). \tag{1}$$

Let R be a finite and X be an arbitrary configuration. The interaction energy of R and X is

$$I(R,X)=\sum_{\mathbf{r}\in R}I(\mathbf{r},X)=\sum_{\mathbf{r}\in R}\sum_{\mathbf{x}\in X}\varphi(\mathbf{r}-\mathbf{x}), \tag{2}$$

and the energy of R in the field of X is

$$U(R|X)=U(R)+I(R,X). \tag{3}$$

If X is an infinite configuration, the infinite sum in (2) must be convergent. This imposes conditions on both X and φ, and the stronger the condition on X, the weaker it can be on φ. For example, one may ask $I(R,X)$ to be finite for *every* X that is locally uniformly finite, meaning the existence of an integer m_X such that the number of particles in a unit cube everywhere in $\mathbb{R}^d$ stays below m_X. This was our choice in Ref. 1; the corresponding condition on the interaction is strong temperedness which for a bounded φ reads

$$\sum_{\mathbf{x}\in X}|\varphi(\mathbf{x})|<\infty \tag{4}$$

for any locally uniformly finite X.

Definition: Given a real μ, X is a ground state configuration of φ for chemical potential μ (a μGSC) if for any bounded domain Λ and any configuration R

$$U(R\cap\Lambda|X\setminus\Lambda)-\mu N_{R\cap\Lambda}\geq U(X\cap\Lambda|X\setminus\Lambda)-\mu N_{X\cap\Lambda}, \tag{5}$$

where $X\cap\Lambda$ and $X\setminus\Lambda$ are parts of X inside and outside Λ, respectively. X is a ground state configuration (GSC) if (5) holds true for every R such that $N_{R\cap\Lambda}=N_{X\cap\Lambda}$.

A seemingly more general, but actually equivalent definition is as follows. X is a μGSC (respectively, X is a GSC) if for any finite part X_f of X and any finite R (respectively, any R such that $N_R=N_{X_f}$),

$$U(R|X\setminus X_f)-\mu N_R\geq U(X_f|X\setminus X_f)-\mu N_{X_f}. \tag{6}$$

If φ is strongly tempered, we can—at least in principle—test any locally uniformly finite X to be, or not, a GSC according to (6). Ground states of interactions that violate condition (4), as those between ions in metals mediated by the Friedel oscillation of the conduction electrons, can be defined only within a more restricted set of configurations. Intuitively, ground states cannot be arbitrary sets of points, they are arrangements with some good averaging (ergodic) property. Specifically, we shall look for them only among periodic configurations and their unions. Simultaneously, the infinite sums appearing in (3) will be suitably interpreted.

A Bravais (direct) lattice $B=\{\Sigma_{\alpha=1}^d n_\alpha\mathbf{a}_\alpha|\mathbf{n}\in\mathbb{Z}^d\}$ is 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. The dual (reciprocal) of B is the Bravais lattice $B^*=\{\Sigma n_\alpha\mathbf{b}_\alpha|\mathbf{n}\in\mathbb{Z}^d\}$ where $\mathbf{a}_\alpha\cdot\mathbf{b}_\beta=2\pi\delta_{\alpha\beta}$. The nearest-neighbor distances in B and B^* are denoted by r_B and q_{B^*}, respectively. The latter is related to the density of B via $\rho(B)=c_{\text{“}B\text{”}}(q_{B^*})^d$, where $c_{\text{“}B\text{”}}$ is determined by the aspect ratios and angles of the primitive cell of B. (Notational remark: B and B^* will always refer to specific Bravais lattices as given above. “B” refers to the family of all Bravais lattices of the type of B, characterized by dimensionless quantities. “B” may take on the value bcc, fcc, simple cubic, and so on.) We shall look for GSCs of the form $X=\cup_{j=1}^J(B_j+\mathbf{y}_j)$ where B_j are Bravais lattices and $B_j+\mathbf{y}_j$ is B_j shifted by the vector $\mathbf{y}_j$. We shall refer to configurations of this form as unions of periodic configurations. If $J=1$, X is a Bravais lattice. If $B_j=B$ for each j then X is periodic. If at least two different Bravais lattices are involved in the union then X is either

periodic or aperiodic, and may contain overlapping points that are to be counted with repetition. The density of X is $\rho(X)=\sum_{j=1}^{J}\rho(B_j)$. Now

$$I(\mathbf{r},X)=\sum_{j=1}^{J} I(\mathbf{r}-\mathbf{y}_j,B_j), \tag{7}$$

so the sum to be interpreted is

$$I(\mathbf{r},B)=\sum_{\mathbf{R}\in B}\varphi(\mathbf{r}+\mathbf{R})=\sum_{\mathbf{n}\in\mathbb{Z}^d}\varphi\left(\mathbf{r}+\sum_{\alpha=1}^{d} n_\alpha \mathbf{a}_\alpha\right). \tag{8}$$

The interaction φ will be defined as the inverse Fourier transform of a function $\hat{\varphi}\in L^1(\mathbb{R}^d)$ that vanishes outside the ball of radius K_0: $\varphi(\mathbf{r})=(2\pi)^{-d}\int_{k<K_0}\hat{\varphi}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}d\mathbf{k}$. Then φ is continuous and all its derivatives exist and are also continuous functions decaying at infinity; in fact, $\varphi(\mathbf{r})$ is an entire function of $\mathbf{r}$.[11] By definition,

$$\sum_{\mathbf{R}\in B}\varphi(\mathbf{r}+\mathbf{R})=\lim_{\varepsilon\downarrow 0}\sum_{\mathbf{R}\in B} e^{-\varepsilon|\mathbf{r}+\mathbf{R}|^2}\varphi(\mathbf{r}+\mathbf{R}) \tag{9}$$

provided that the limit exists. In our case a weaker, e.g., exponential, tempering would suffice and give the same result; the Gaussian tempering is more convenient to work with in an arbitrary dimension. Note that the sum on the right-hand side is absolutely convergent for any $\varepsilon>0$. It is easily seen that whenever the sum in (8) is absolutely convergent, Eq. (9) yields the same result. This is the case of all the examples given in Ref. 1. In the absence of absolute convergence, the sum (8) can still be conditionally convergent; e.g., with some mild additional assumption on $\hat{\varphi}$ one can show that

$$I(\mathbf{r},B)=\lim_{N_1,\ldots,N_d\to\infty}\sum_{\mathbf{n}\in\mathbb{Z}^d,|n_\alpha|<N_\alpha}\varphi\left(\mathbf{r}+\sum_{\alpha=1}^{d} n_\alpha \mathbf{a}_\alpha\right) \tag{10}$$

exists and agrees with the result suggested by the Poisson summation formula. However, the proof of this formula is simpler with the definition (9).

Theorem: Let $\hat{\varphi}\in L^1(\mathbb{R}^d)$ be a real function with the following properties:

(1) $\hat{\varphi}$ is continuous at the origin,
(2) $\hat{\varphi}(-\mathbf{k})=\hat{\varphi}(\mathbf{k})$,
(3) $\hat{\varphi}\geq 0$, and
(4) there is some K_0 such that $\hat{\varphi}(\mathbf{k})=0$ for $|\mathbf{k}|>K_0$.

(i) Define $\varphi(\mathbf{r})=(2\pi)^{-d}\int\hat{\varphi}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}d\mathbf{k}$. Choose Bravais lattices $B_1,\ldots,B_J$ such that each $q_{B_j^*}\geq K_0$, where equality is allowed only if $\hat{\varphi}$ is continuous at $|\mathbf{k}|=K_0$. Then $X=\cup_{j=1}^{J}(B_j+\mathbf{y}_j)$ is a GSC of φ for arbitrary translations $\mathbf{y}_j$ and it is also a μGSC for $\mu=\rho(X)\hat{\varphi}(\mathbf{0})-\frac{1}{2}\varphi(\mathbf{0})$. The energy per unit volume of X is $e(X)=\epsilon(\rho(X))$ where

$$\epsilon(\rho)=\frac{1}{2}\rho[\rho\hat{\varphi}(\mathbf{0})-\varphi(\mathbf{0})] \tag{11}$$

is the minimum of the energy density among unions of periodic configurations of density ρ. GSCs of the above properties exist in a semi-infinite density interval $[\rho_d,\infty)$.

(ii) If φ is strongly tempered and X is locally uniformly finite with existing $\rho(X)\geq\rho_d$ and $e(X)>\epsilon(\rho(X))$, then X is not a GSC. If φ is not strongly tempered but the limit (10) on Bravais lattices exists, then any union X of periodic configurations with $\rho(X)\geq\rho_d$ and $e(X)>\epsilon(\rho(X))$ is not a GSC.

(iii) Let $r_0\leq\gamma_d/K_0$, where $\gamma_1=2\pi$, $\gamma_2=4\pi/\sqrt{3}$ and $\gamma_3=\sqrt{6}\pi$, and let ψ be a real function such that $\psi(\mathbf{r})\in[0,\infty]$ and $\psi(\mathbf{r})=0$ for $r\geq r_0$. If $r_B\geq r_0$ and $q_{B^*}\geq K_0$, then B is a GSC and a μGSC of $\varphi+\psi$ with μ and $e(B)$ given above, not depending on ψ. GSCs of the above properties exist in a density interval $[\rho_d,\rho_d']$.

Remarks: (1) Compared with the theorem of Ref. 1, the conditions on φ are formulated uniquely via $\hat{\varphi}$, and are considerably weaker. For instance, $\hat{\varphi}$ or its derivative can be discontinuous at K_0. Here are two examples in three dimensions: $\hat{\varphi}(\mathbf{k})\equiv 1$ for $k<K_0$ yields ($k=|\mathbf{k}|$, $r=|\mathbf{r}|$)

$$\varphi(\mathbf{r})=-(K_0/2\pi^2)\cos K_0 r/r^2+(1/2\pi^2)\sin K_0 r/r^3, \tag{12}$$

while with $\hat{\varphi}(\mathbf{k})=1-k/K_0$ for $k<K_0$ we obtain

$$\varphi(\mathbf{r})=\frac{\cos(K_0 r+\pi/2)}{2\pi^2 r^3}+\frac{1-\cos K_0 r}{\pi^2 K_0 r^4}. \tag{13}$$

Both are conditionally summable on Bravais lattices [if B^* has no point on the sphere $|\mathbf{K}|=K_0$, in the case of (12)], as defined in Eq. (10).

(2) We proved in Ref. 1 that the condition $q_{B^*}\geq K_0$ can be satisfied only if $\rho\geq\rho_d$, a dimension-dependent threshold density at which $q_{B^*}=K_0$ for a unique Bravais lattice B, and this is the unique periodic GSC; in particular, $\rho_3=K_0^3/8\sqrt{2}\pi^3$ and the lattice is the bcc one. The above form of the theorem shows that for $\rho_d\leq\rho<2\rho_d$ no union is available, only Bravais lattices can be GSCs. In Ref. 1 we gave also the densities of some Bravais lattices B at which $q_{B^*}=K_0$. Recalling these values,

$$\rho_{\mathrm{bcc}}=\rho_3<\rho_{\mathrm{fcc}}=\frac{4\sqrt{2}}{3\sqrt{3}}\rho_3=1.089\rho_3$$

$$<\rho_{\mathrm{sh}}=\sqrt{\frac{3}{2}}\rho_3<\rho_{\mathrm{sc}}=\sqrt{2}\rho_3 \tag{14}$$

(sh represents simple hexagonal with $c/a=\sqrt{3}/2$, sc represents simple cubic), one can see that all the high-symmetry Bravais lattices appear as GSCs between ρ_3 and $2\rho_3$. Also, if $\rho(Z)$ denotes the density of a metal of valency Z then, in the free-electron approximation and supposing a spherical Fermi surface of radius $k_F=K_0/2$, $\rho(Z)=(\sqrt{2}\pi/3Z)\rho_3=(1.481/Z)\rho_3$ which for $Z=1$ is in this interval. In general, in the interval $n\rho_d\leq\rho<(n+1)\rho_d$ the ground state configurations are unions of at most n Bravais lattices, each of density $\geq\rho_d$. Thus, the simplest aperiodic GSCs, unions of two incommensurate Bravais lattices, appear only if $\rho\geq 2\rho_d$. For example, in three dimensions at $2\rho_3$ they are the unions of two bcc lattices rotated and possibly shifted with respect to each other.

(3) The family of all the GSCs of φ above the density ρ_d is closed on unions. This is obvious from the present formulation, because the union of two GSCs of the form given in

the theorem is a configuration of the same form, so it is necessarily also a GSC. Recall from Ref. 1 that a periodic configuration X is called B-periodic if $X=\cup_{j=1}^{J}(B+\mathbf{y}_j)$ and B is chosen so as to minimize J. If X_m are B_m-periodic configurations then $\cup X_m$ is periodic if and only if $B=\cap B_m$ is a d-dimensional Bravais lattice. Because $B\subseteq B_m$, $B^*\supseteq B_m^*$ and $q_{B^*}\leq q_{B_m^*}$. It follows that a B-periodic configuration $X=\cup_{j=1}^{J}(B+\mathbf{y}_j)$ can be a GSC even if $q_{B^*}<K_0$, provided that it can be written also as $X=\cup_{j=1}^{J'}(B_j+\mathbf{y}'_j)$, where $q_{B_j^*}\geq K_0$ for $j=1,\ldots,J'$. This means that on average the B_j's are denser than B and thus $J'<J$. Logically, if we permit different Bravais lattices to occur in the union forming a periodic configuration, the number of components may be decreased.

(4) A μGSC is, by definition, also a GSC because it satisfies a stronger condition. Therefore, in the theorem it would have been enough to say that X or B is a μGSC. We wanted to emphasize that the theorem strengthens that of Ref. 1 by stating that the opposite is also true: a GSC is always a μGSC, even if $\hat{\varphi}(\mathbf{0})=0$ and thus φ is not superstable. In the latter case $\mu=-\frac{1}{2}\varphi(\mathbf{0})$, independently of the density of the ground state configuration.

(5) Assertion (ii) of the theorem extends to a larger class of configurations and pair potentials earlier results by Sewell[16] and Sinai[17] on the absence of metastability for strongly tempered interactions. Following the usual definition,[17] we apply the term "ground state configuration" as a synonym of a locally stable configuration. Thus, a GSC could be globally unstable, meaning that by some perturbation involving infinitely many particles its energy density could be decreased. Such a GSC might be called metastable. However, we must precise the kind of infinite perturbations we allow. If the particle density is allowed to vary, usually the absolute minimum of the energy density is attained at a single value of ρ, and all GSCs of a different density should be considered metastable. In this sense, the unique stable GSC of an everywhere positive interaction is the vacuum, and for the interactions φ studied in this paper the globally stable GSCs are the μGSCs belonging to $\mu=0$ [hence, to $\rho=\varphi(\mathbf{0})/2\hat{\varphi}(\mathbf{0})$, if this value is finite and not smaller than ρ_d]. We adopt a more restrictive definition of metastability, not allowing the density to vary. Then the configurations characterized by the theorem as GSCs are not metastable because their energy density is the attainable minimum for their density, and no other configuration (within the specified class) can be a metastable ground state.

(6) A sufficient condition for φ to be strongly tempered is that $|\varphi(\mathbf{r})|\leq Cr^{-d-\eta}$ for $r>r'$, where C, η, and r' are some positive numbers. In our case this holds, for example, if besides conditions (1)–(4), $\hat{\varphi}$ is 3 times differentiable, see Eq. (9) of Ref. 1.

(7) Point (iii) of the theorem needs more of an explanation than a formal proof. When we ask $r_B\geq r_0$, we limit the role of ψ to reducing the degeneracy of the GSCs of φ. The largest allowed range of ψ, $r_0=\gamma_d/K_0$, equals the nearest-neighbor distance of the unique GSC of φ at the density ρ_d: the uniform chain, the triangular lattice, and the bcc lattice for $d=1$, 2, and 3, respectively. The theorem makes no prediction if $r_0>\gamma_d/K_0$, because no Bravais lattice satisfies both conditions $r_B>\gamma_d/K_0$ and $q_{B^*}\geq K_0$. This is an obvious consequence of $r_Bq_{B^*}=2\pi$ in one dimension, and of

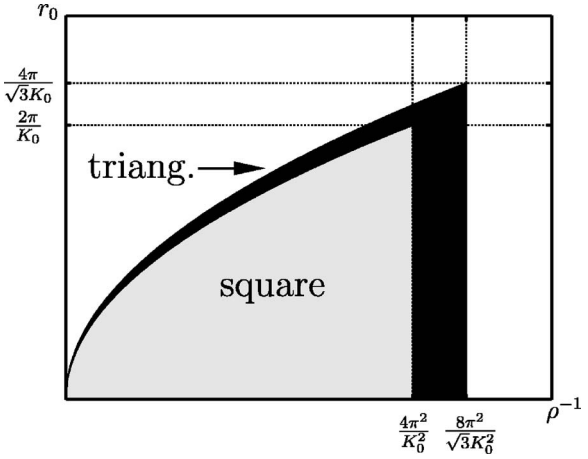

FIG. 1. Stability of two-dimensional lattices. The stability intervals of the triangular and square lattices are obtained as horizontal cuts of the respective domains.

$$\gamma_d=\max_B r_Bq_{B^*}=\begin{cases}4\pi/\sqrt{3} & (d=2),\\ \sqrt{6}\pi & (d=3),\end{cases} \tag{15}$$

with the maximum attained if B is the triangular lattice in two, and the bcc (or fcc) lattice in three dimensions. We prove (15) in the next section, and suppose henceforth that $r_0K_0\leq\gamma_d$. For a given lattice type "B", $r_Bq_{B^*}=\gamma_{\text{"}B\text{"}}=\gamma_{\text{"}B^*\text{"}}$, independent of the density. This implies that the simultaneous inequalities $r_B\geq r_0$ and $q_{B^*}\geq K_0$ hold in a (closed) interval of the density, whose lower and upper boundaries are implicitly determined by $q_{B^*}=K_0$ and $r_B=r_0$, respectively. If ρ is in this "stability interval" $I_{\text{"}B\text{"}}$, then B is a GSC of $\varphi+\psi$, with energy density $e(B)=\epsilon(\rho)$. If ρ is not in $I_{\text{"}B\text{"}}$, then $e(B)>\epsilon(\rho)$ (provided the strict positivity of $\hat{\varphi}$ for $k<K_0$ and of ψ for $r<r_0$, that we suppose now), and B is surely not a GSC of $\varphi+\psi$ if ρ is still in the stability interval of some other Bravais lattice $\tilde{B}$: In this case $\tilde{B}$ is a GSC with energy density $e(\tilde{B})=\epsilon(\rho)$, and due to the absence of metastability, B cannot be a GSC. $I_{\text{"}B\text{"}}$ shrinks to a single point if $r_0=\gamma_{\text{"}B\text{"}}/K_0$ and disappears if $r_0>\gamma_{\text{"}B\text{"}}/K_0$. In two dimensions $\gamma_2=\gamma_{\text{tr}}$, so this may happen with any Bravais lattice other than the triangular one. Because the triangular lattice is self-dual, at a given density it has the largest q_{B^*} *and* the largest r_B among the two-dimensional Bravais lattices. Therefore its stability interval

$$I_{\text{tr}}=[\rho_2,\rho(r_{\text{tr}}=r_0)]\equiv[\rho_2,\rho_2']=\left[\frac{\sqrt{3}K_0^2}{8\pi^2},\frac{2}{\sqrt{3}r_0^2}\right] \tag{16}$$

contains in its interior the stability intervals of all the other Bravais lattices. Figure 1 shows the stability intervals of the triangular and the square lattices for all allowed values of r_0. If ρ falls into I_{tr} but outside $I_{\text{"}B\text{"}}$, then B is certainly not a GSC of $\varphi+\psi$ at this density. In particular, at the two ends of I_{tr} the only GSC is the triangular lattice. The uniqueness at the upper value $\rho_2'=2/\sqrt{3}r_0^2$ is new, and is due to ψ. The

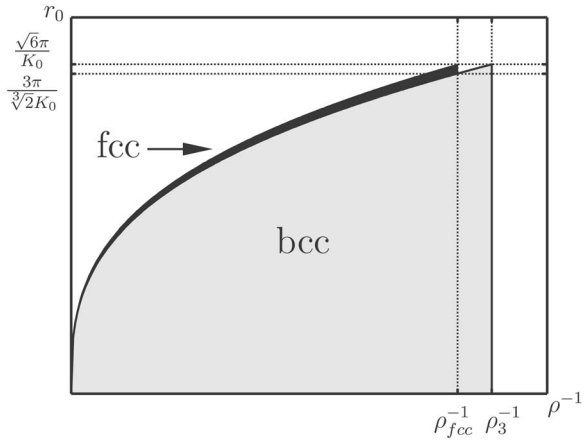

FIG. 2. Stability of three-dimensional lattices. The stability intervals of the bcc and fcc lattices are obtained as horizontal cuts of the respective domains.

situation in three dimensions is more complicated, because $\gamma_3=\gamma_{\rm bcc}=\gamma_{\rm fcc}$. From the expressions

$$r_{\rm bcc}(\rho)=\sqrt{3}/(4\rho)^{1/3},\quad r_{\rm fcc}(\rho)=(\sqrt{2}/\rho)^{1/3} \tag{17}$$

of the nearest-neighbor distances one can see that the stability intervals for the bcc and fcc lattices are

$$I_{\rm bcc}=\left[\frac{K_0^3}{8\sqrt{2}\pi^3},\frac{3\sqrt{3}}{4r_0^3}\right],\quad I_{\rm fcc}=\left[\frac{K_0^3}{6\sqrt{3}\pi^3},\frac{\sqrt{2}}{r_0^3}\right], \tag{18}$$

the lower boundaries being $\rho_3\equiv\rho_{\rm bcc}$ and $\rho_{\rm fcc}$, respectively, cf. Eq. (14). Because at a given density the bcc lattice has the largest q_{B^*} and the fcc the largest r_B, the stability interval of any Bravais lattice is between ρ_3 and $\rho_3'=\sqrt{2}/r_0^3$. According to the argument given above, at ρ_3 and ρ_3' the ground state is unique; especially, *at* $\rho=\sqrt{2}/r_0^3$ *the unique GSC is the fcc lattice*. The intervals $I_{\rm bcc}$ and $I_{\rm fcc}$ only partially overlap, and may not overlap at all: if $3\pi/2^{1/3}<r_0K_0\le\sqrt{6}\pi$, $I_{\rm bcc}$ and $I_{\rm fcc}$ are disjoint. For $r_0<\sqrt{6}\pi/K_0$ the stability intervals of other Bravais lattices fill the gap. At $r_0=\sqrt{6}\pi/K_0$, $I_{\rm bcc}$ and $I_{\rm fcc}$ shrink to a single point, $\rho_{\rm bcc}$ and $\rho_{\rm fcc}$, respectively, and for densities in between no Bravais lattice satisfies both conditions $q_{B^*}\ge K_0$ and $r_B\ge r_0$. In this interval the ground state is probably unique and changes continuously from bcc to fcc as the density increases. In Fig. 2 we present the stability intervals of the bcc and the fcc lattices for all the allowed values of r_0.

The GSCs of φ will be found by applying the following extension of the Poisson summation formula.

Lemma: Let $\hat{\varphi}\in L^1(\mathbb{R}^d)$ be a function of bounded support, which is continuous at the origin. Let $\varphi(\mathbf{r})=(2\pi)^{-d}\int\hat{\varphi}(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}d\mathbf{k}$. Choose a Bravais lattice B such that $\hat{\varphi}$ is continuous at every $\mathbf{K}$ in B^*. Then

$$\lim_{\varepsilon\downarrow 0}\sum_{\mathbf{R}\in B}e^{-\varepsilon|\mathbf{r}+\mathbf{R}|^2}\varphi(\mathbf{r}+\mathbf{R})=\rho(B)\sum_{\mathbf{K}\in B^*}\hat{\varphi}(\mathbf{K})e^{i\mathbf{K}\cdot\mathbf{r}}, \tag{19}$$

implying the existence of the limit.

Observe that the sum on the right-hand member has only a finite number of nonzero terms, hence for any B the continuity of $\hat{\varphi}$ is to be checked only in a finite number of points. In particular, for any B dense enough the only point of B^* inside the support of $\hat{\varphi}$ is the origin, where $\hat{\varphi}$ is continuous. This is precisely the fact we shall use in the proof of the theorem.

III. PROOFS

A. Proof of the lemma

Let

$$\delta_\varepsilon(\mathbf{k})=(4\pi\varepsilon)^{-d/2}e^{-k^2/4\varepsilon}. \tag{20}$$

First, we show that

$$\sum_{\mathbf{R}\in B}e^{-\varepsilon|\mathbf{r}+\mathbf{R}|^2}\varphi(\mathbf{r}+\mathbf{R})=\rho(B)\sum_{\mathbf{K}\in B^*}(\hat{\varphi}*\delta_\varepsilon)(\mathbf{K})e^{i\mathbf{K}\cdot\mathbf{r}} \tag{21}$$

for any $\varepsilon>0$. The argument is essentially the same as the one we used to prove the lemma of Ref. 1. Because $\varphi(\mathbf{r})$ is an entire function of $\mathbf{r}$ decaying at infinity, both $e^{-\varepsilon r^2}\varphi(\mathbf{r})$ and its Fourier transform $\hat{\varphi}*\delta_\varepsilon$ are functions of rapid decrease.[15] Therefore, the infinite sums on both sides of Eq. (21) are absolutely convergent and the convergence is uniform in $\mathbf{r}$. So both sums define continuous functions, that are periodic with periods $\mathbf{R}\in B$ and have the same Fourier coefficients. Indeed, multiplying Eq. (21) by $e^{-i\mathbf{K}\cdot\mathbf{r}}$ and integrating by terms over the unit cell of volume $\rho(B)^{-1}$, on the left-hand side after summation we obtain $(\hat{\varphi}*\delta_\varepsilon)(\mathbf{K})$, which is also the trivial result on the right-hand side. Because of the completeness of the system $\{e^{i\mathbf{K}\cdot\mathbf{r}}|\mathbf{K}\in B^*\}$ in the Banach space of integrable functions on the unit cell of B, the two continuous periodic functions coincide everywhere.

Next, we prove that the integrability of $\hat{\varphi}$ and its continuity at $\mathbf{K}$ imply

$$\lim_{\varepsilon\to 0}(\hat{\varphi}*\delta_\varepsilon)(\mathbf{K})=\hat{\varphi}(\mathbf{K}). \tag{22}$$

Fix any $\eta>0$ and write

$$(\hat{\varphi}*\delta_\varepsilon)(\mathbf{K})=\int_{q<\eta}\hat{\varphi}(\mathbf{K}-\mathbf{q})\delta_\varepsilon(\mathbf{q})d\mathbf{q}+\int_{q>\eta}\hat{\varphi}(\mathbf{K}-\mathbf{q})\delta_\varepsilon(\mathbf{q})d\mathbf{q}\equiv J_{\varepsilon,<\eta}+J_{\varepsilon,>\eta}. \tag{23}$$

If ε is small enough then $\delta_\varepsilon(\mathbf{q})<1$ for $q>\eta$, and in $J_{\varepsilon,>\eta}$ the integrand can be bounded above by $|\hat{\varphi}(\mathbf{K}-\mathbf{q})|$. Thus, due to the dominated convergence theorem the limit and the integration can be interchanged, resulting $\lim_{\varepsilon\to 0}J_{\varepsilon,>\eta}=0$, because $\lim_{\varepsilon\to 0}\delta_\varepsilon(\mathbf{q})=0$ for $q>\eta$. On the other hand,

$$J_{\varepsilon,<\eta} = \hat{\varphi}(\mathbf{K}) \int_{q<\eta} \delta_\varepsilon(\mathbf{q}) d\mathbf{q} + \int_{q<\eta} [\hat{\varphi}(\mathbf{K}-\mathbf{q}) - \hat{\varphi}(\mathbf{K})] \delta_\varepsilon(\mathbf{q}) d\mathbf{q}. \quad (24)$$

Now $\lim_{\varepsilon\to 0}\int_{q<\eta}\delta_\varepsilon(\mathbf{q})d\mathbf{q}=1$ and

$$\left| \int_{q<\eta} [\hat{\varphi}(\mathbf{K}-\mathbf{q}) - \hat{\varphi}(\mathbf{K})] \delta_\varepsilon(\mathbf{q}) d\mathbf{q} \right| \le \sup_{q<\eta} |\hat{\varphi}(\mathbf{K}-\mathbf{q}) - \hat{\varphi}(\mathbf{K})|. \quad (25)$$

Combining the above equations,

$$\lim_{\varepsilon\to 0} |(\hat{\varphi} * \delta_\varepsilon)(\mathbf{K}) - \hat{\varphi}(\mathbf{K})| \le \sup_{q<\eta} |\hat{\varphi}(\mathbf{K}-\mathbf{q}) - \hat{\varphi}(\mathbf{K})|, \quad (26)$$

from which the result follows by letting η go to zero.

Finally, using the fact that the different sums involving $\hat{\varphi}(\mathbf{K})$ [but not $(\hat{\varphi}*\delta_\varepsilon)(\mathbf{K})$!] are finite, we find

$$\lim_{\varepsilon\to 0} \left| \sum_{\mathbf{K}\in B^*} [(\hat{\varphi} * \delta_\varepsilon)(\mathbf{K}) - \hat{\varphi}(\mathbf{K})] e^{i\mathbf{K}\cdot\mathbf{r}} \right| \le \sum_{\mathbf{K}\in B^*} \sup_{q<\eta} |\hat{\varphi}(\mathbf{K}-\mathbf{q}) - \hat{\varphi}(\mathbf{K})|, \quad (27)$$

holding for all $\eta>0$. Thus, we can conclude that the left-hand side is indeed zero. This completes the proof of the lemma.

B. Proof of Eq. (15)

The proof is based on the well-known fact that $2\pi/q_{B^*}$ is the largest distance between neighboring lattice lines ($d=2$) or planes ($d=3$) of B, see e.g., Ref. 18. The way we proceed is to consider all the types of Bravais lattices simultaneously and to select, through a sequence of choices, the vectors $\mathbf{a}_i$ that define the maximizer of $r_B q_{B^*}$. Let B be any two-dimensional Bravais lattice. Choose $\mathbf{a}_1$ among the shortest vectors of B, hence $a_1=r_B$. The lattice line parallel to $\mathbf{a}_1$ is a line of largest density, therefore the largest distance between neighboring lines is measured perpendicular to $\mathbf{a}_1$. The other primitive vector, $\mathbf{a}_2$ is selected among the shortest vectors not collinear with $\mathbf{a}_1$ and making an acute angle α with $\mathbf{a}_1$. Then $\alpha\ge\pi/3$ (otherwise $\mathbf{a}_1-\mathbf{a}_2$ would be shorter, and should replace $\mathbf{a}_2$), and $2\pi/q_{B^*}=a_2\sin\alpha$ (thus, $b_2=q_{B^*}$). Therefore,

$$r_B q_{B^*} = \frac{2\pi a_1}{a_2 \sin\alpha}, \quad (28)$$

whose maximum on the condition that $a_2\ge a_1$ and $\pi/3\le\alpha\le\pi/2$ is $4\pi/\sqrt{3}$, attained with the choice $a_2=a_1$ and $\alpha=\pi/3$, characteristic to the triangular lattice.

In three dimensions, given B, let P be a lattice plane of highest density, containing the origin. Let $\mathbf{a}_1$ be one of the shortest lattice vectors in the plane, and choose $\mathbf{a}_2$ among the shortest lattice vectors in P not collinear with $\mathbf{a}_1$ and making an acute angle α_{12} with it; so we have $a_1\le a_2$ and, as argued above, $\pi/3\le\alpha_{12}\le\pi/2$. Because P is of highest density, the largest distance among lattice planes can be measured perpendicular to it. Correspondingly, $q_{B^*}=b_3$. Choose $\mathbf{a}_3$ among the shortest lattice vectors not contained in P and making an acute angle with at least one of $\mathbf{a}_1$ or $\mathbf{a}_2$. One of the angles, α_{13} of $\mathbf{a}_1$ and $\mathbf{a}_3$ or α_{23} of $\mathbf{a}_2$ and $\mathbf{a}_3$, can indeed be obtuse. However, if it is obtuse, we replace B by B^* in the line of reasoning and continue with three acute angles: this will not influence the validity of Eq. (15). We must examine two cases. First, suppose that $a_1=r_B$. Then

$$r_B q_{B^*} = \frac{2\pi a_1 |\mathbf{a}_1\times\mathbf{a}_2|}{|\mathbf{a}_3\cdot(\mathbf{a}_1\times\mathbf{a}_2)|} = \frac{2\pi a_1}{a_3\sin\alpha}, \quad (29)$$

where α is the angle of $\mathbf{a}_3$ to P. To maximize $r_B q_{B^*}$, we choose $a_3=a_1=r_B$ and then α to be minimum. None of α_{13} and α_{23} can be smaller than α_{12}, otherwise the density of the plane spanned by $\mathbf{a}_3$ with either $\mathbf{a}_1$ or $\mathbf{a}_2$ would be higher than that of P. Therefore, the smallest α can be attained if $\mathbf{a}_3$ is in the bisector plane of α_{12} and $\alpha_{13}=\alpha_{23}=\alpha_{12}=\pi/3$. But then a_2 cannot be larger than a_1, otherwise, again, P was not a plane of maximum density. Thus, we conclude that $a_1=a_2=a_3=r_B$ and $\alpha_{12}=\alpha_{23}=\alpha_{31}=\pi/3$, specifying the fcc lattice. The other case is $r_B=a_3<a_1$. Then again $r_B q_{B^*}=2\pi/\sin\alpha$, but now α cannot be as small as before, otherwise the density of a lattice plane containing $\mathbf{a}_3$ would be larger than that of P. Thus, the maximum of $r_B q_{B^*}$ is indeed attained on the fcc-bcc pair. Its value, $\sqrt{6}\pi$, is easy to compute.

C. Proof of the theorem, (i)

Let $X=\cup_{j=1}^J (B_j+\mathbf{y}_j)$, $X_f\subset X$ finite, and let R be any finite configuration. If $\hat{\varphi}$ is continuous at each point of every B_j^* then, making use of the definitions (1)–(3) and (9) and the lemma,

$$\begin{aligned} U(R|X\setminus X_f) &= N_R[\hat{\varphi}(\mathbf{0})\rho(X) - \varphi(\mathbf{0})/2] \\ &+ \int \hat{\varphi}(\mathbf{k}) \left(\left| \sum_{\mathbf{r}\in R} e^{i\mathbf{k}\cdot\mathbf{r}} \right|^2 \right. \\ &\left. - 2\sum_{\mathbf{r}\in R} e^{i\mathbf{k}\cdot\mathbf{r}} \sum_{\mathbf{x}\in X_f} e^{-i\mathbf{k}\cdot\mathbf{x}} \right) \frac{d\mathbf{k}}{2(2\pi)^d} \\ &+ \sum_{j=1}^J \rho(B_j) \sum_{\mathbf{0}\ne\mathbf{K}\in B_j^*} \hat{\varphi}(\mathbf{K}) e^{-i\mathbf{K}\cdot\mathbf{y}_j} \sum_{\mathbf{r}\in R} e^{i\mathbf{K}\cdot\mathbf{r}}. \end{aligned} \quad (30)$$

Subtracting the corresponding expression in which X_f replaces R, we find

$$\begin{aligned} &U(R|X\setminus X_f) - \mu N_R - U(X_f|X\setminus X_f) + \mu N_{X_f} \\ &= (N_{X_f} - N_R)[\mu + \varphi(\mathbf{0})/2 - \hat{\varphi}(\mathbf{0})\rho(X)] \\ &+ \int \hat{\varphi}(\mathbf{k}) \left| \sum_{\mathbf{r}\in R} e^{i\mathbf{k}\cdot\mathbf{r}} - \sum_{\mathbf{x}\in X_f} e^{i\mathbf{k}\cdot\mathbf{x}} \right|^2 \frac{d\mathbf{k}}{2(2\pi)^d} \\ &+ \sum_{j=1}^J \rho(B_j) \sum_{\mathbf{0}\ne\mathbf{K}\in B_j^*} \hat{\varphi}(\mathbf{K}) e^{-i\mathbf{K}\cdot\mathbf{y}_j} \left(\sum_{\mathbf{r}\in R} e^{i\mathbf{K}\cdot\mathbf{r}} - \sum_{\mathbf{x}\in X_f} e^{i\mathbf{K}\cdot\mathbf{x}} \right). \end{aligned} \quad (31)$$

Suppose now that each $q_{B_j^*} \geq K_0$, where equality is allowed only if $\hat{\varphi}(\mathbf{k})=0$ at $|\mathbf{k}|=K_0$. Any such set of B_j's satisfies the continuity assumption. Indeed, $\hat{\varphi}$ is continuous at $\mathbf{K}=\mathbf{0}$ and, because $|\mathbf{K}| \geq K_0$ for every nonzero $\mathbf{K}$ in $\cup_{j=1}^{J} B_j^*$, $\hat{\varphi}$ is continuous and takes on zero in all these points. Equation (31) is, therefore, valid, and the last term on its right-hand side vanishes for all R. The first term can be made zero either by choosing $N_R=N_{X_f}$ or by setting $\mu=\hat{\varphi}(\mathbf{0})\rho(X)-\varphi(\mathbf{0})/2$. Because $\hat{\varphi} \geq 0$, these choices prove that X is indeed a GSC and a μGSC of φ.

Next, we compute the energy density $e(X)$ of X with each $q_{B_j^*} \geq K_0$. From Eq. (7) and the lemma,

$$I(\mathbf{x},X) = \rho(X)\hat{\varphi}(\mathbf{0}). \tag{32}$$

Furthermore, if Q_L denotes the cube of side L centered at the origin, then

$$\lim_{L\to\infty} L^{-d} \sum_{\mathbf{x}\in X\cap Q_L} 1 = \rho(X). \tag{33}$$

With Eqs. (32) and (33),

$$\begin{aligned} e(X) &= \frac{1}{2}\lim_{L\to\infty} L^{-d} \sum_{\mathbf{x}\in X\cap Q_L} \sum_{\mathbf{x}\neq\mathbf{x}'\in X} \varphi(\mathbf{x}-\mathbf{x}') \\ &= \frac{1}{2}\lim_{L\to\infty} L^{-d} \sum_{\mathbf{x}\in X\cap Q_L} [I(\mathbf{x},X)-\varphi(\mathbf{0})] \\ &= -\frac{1}{2}\rho(X)\varphi(\mathbf{0}) + \frac{1}{2}\rho(X)^2\hat{\varphi}(\mathbf{0}) = \epsilon(\rho(X)). \end{aligned} \tag{34}$$

Here the first two equalities define the energy density of a general configuration, only the third one is specific to a GSC. We now prove that $\epsilon(\rho)$ is the minimum of $e(X)$ within the set of unions of periodic configurations of density ρ. As earlier, we write an arbitrary (periodic or aperiodic) union of periodic configurations in the form $X=\cup_{j=1}^{J}(B_j+\mathbf{y}_j)$. Computing $I(\mathbf{x},X)$ with the help of Eq. (19), inserting it into the definition (34) of $e(X)$ and separating the $\mathbf{K}=\mathbf{0}$ term we find

$$\begin{aligned} e(X) = \epsilon(\rho(X)) &+ \frac{1}{2}\sum_{i,j=1}^{J} \rho(B_i) \\ &\times \sum_{\mathbf{0}\neq\mathbf{K}\in B_i^*} \hat{\varphi}(\mathbf{K}) e^{i\mathbf{K}\cdot(\mathbf{y}_j-\mathbf{y}_i)} \lim_{L\to\infty} L^{-d} \sum_{\mathbf{R}\in B_j\cap(Q_L-\mathbf{y}_j)} e^{i\mathbf{K}\cdot\mathbf{R}}. \end{aligned} \tag{35}$$

The limit can be evaluated: it yields $\rho(B_j)$ if $\mathbf{K}\in B_i^*\cap B_j^*$ and zero if $\mathbf{K}\in B_i^*\backslash B_j^*$. Hence, we obtain

$$\begin{aligned} e(X) &= \epsilon(\rho(X)) + \frac{1}{2}\sum_{i,j=1}^{J} \rho(B_i)\rho(B_j) \sum_{\mathbf{0}\neq\mathbf{K}\in B_i^*\cap B_j^*} \hat{\varphi}(\mathbf{K}) e^{i\mathbf{K}\cdot(\mathbf{y}_j-\mathbf{y}_i)} \\ &= \epsilon(\rho(X)) + \frac{1}{2}\sum_{\mathbf{0}\neq\mathbf{K}\in\cup B_i^*} \hat{\varphi}(\mathbf{K}) \left| \sum_{j=1}^{J} \chi_{B_j^*}(\mathbf{K})\rho(B_j) e^{i\mathbf{K}\cdot\mathbf{y}_j} \right|^2, \end{aligned} \tag{36}$$

where $\chi_{B_j^*}(\mathbf{K})=1$ if $\mathbf{K}$ is in B_j^* and is zero otherwise. Thus, $e(X) \geq \epsilon(\rho(X))$, as claimed.

D. Proof of the theorem, (ii): absence of metastability

The following proposition makes no use of Fourier transforms, but exploits directly the summability assumptions (4) and (10).

Proposition: (i) Let φ be a strongly tempered pair potential. Let X and Y be locally uniformly finite configurations such that the limits (33) and (34), defining the density and the energy density, exist. If $\rho(X)=\rho(Y)$ but $e(X)>e(Y)$, then X is not a GSC of φ, that is, X does not satisfy the local stability condition (5) restricted to number-preserving perturbations. (ii) If φ is not strongly tempered but summable on Bravais lattices in the sense of Eq. (10), and X and Y are unions of periodic configurations with $\rho(X)=\rho(Y)$ and $e(X)>e(Y)$, then X is not a GSC of φ.

Proof: The proof was already outlined in Ref. 1. Here we give the missing details. (i) In the case of strongly tempered interactions consider the cubes Q_L introduced above. In general, $\Delta_L=N_{X\cap Q_L}-N_{Y\cap Q_L}\neq 0$ but, because $\rho(X)=\rho(Y)$, $\Delta_L=o(L^d)$. Let Y_L be a configuration in Q_L obtained from $Y\cap Q_L$ by adding or deleting $|\Delta_L|$ points so that $N_{Y_L}=N_{X\cap Q_L}$. From the definitions (3) and (34) we deduce

$$U(X\cap Q_L|X\backslash Q_L) = e(X)L^d + \tfrac{1}{2}I(X\cap Q_L, X\backslash Q_L) + o(L^d). \tag{37}$$

On the other hand, by strong temperedness,

$$U(Y_L|X\backslash Q_L) = U(Y\cap Q_L|X\backslash Q_L) + o(L^d),$$

and therefore

$$\begin{aligned} U(Y_L|X\backslash Q_L) = e(Y)L^d &+ I(Y\cap Q_L, X\backslash Q_L) \\ &- \tfrac{1}{2}I(Y\cap Q_L, Y\backslash Q_L) + o(L^d). \end{aligned} \tag{38}$$

To conclude that

$$U(Y_L|X\backslash Q_L) - U(X\cap Q_L|X\backslash Q_L) \asymp [e(Y)-e(X)]L^d < 0$$

for L large enough, we must show that the I terms in Eqs. (37) and (38) are of smaller order, $o(L^d)$. Again, this holds because φ is strongly tempered. For example,

$$\begin{aligned} &L^{-d}|I(X\cap Q_L, X\backslash Q_L)| \\ &\quad = L^{-d}|I(X\cap Q_{L-\sqrt{L}}, X\backslash Q_L) + I(X\cap Q_L\backslash Q_{L-\sqrt{L}}, X\backslash Q_L)| \\ &\quad \leq \rho(X)\left[\sup_{\mathbf{r}} \sum_{\mathbf{x}\in X, |\mathbf{x}-\mathbf{r}|\geq\sqrt{L}} |\varphi(\mathbf{x}-\mathbf{r})| \right. \\ &\qquad \left. + L^{-d/2} \sup_{\mathbf{r}} \sum_{\mathbf{x}\in X} |\varphi(\mathbf{x}-\mathbf{r})| \right] + o(1) \end{aligned}$$

which indeed tends to zero as L goes to infinity. (ii) In the case when φ is not strongly tempered, let $X=\cup_{j=1}^{J}(B_j+\mathbf{y}_j)$ and $Y=\cup_{j=1}^{J'}(B'_j+\mathbf{y}'_j)$, with primitive vectors $\mathbf{a}_{j,\alpha}$ and $\mathbf{a}'_{j,\alpha}$, respectively. Consider the set $\cup_{j=1}^{J}\{\Sigma_\alpha n_\alpha \mathbf{a}_{j,\alpha}+\mathbf{y}_j \,|\, |n_\alpha|<N_\alpha\}$, and let X_f be the union of J' nonoverlapping adjacent translates of this set. Similarly, let R be the union of J nonoverlapping adjacent translates of the set $\cup_{j=1}^{J'}\{\Sigma_\alpha n_\alpha \mathbf{a}'_{j,\alpha}+\mathbf{y}'_j \,|\, |n_\alpha|<N_\alpha\}$. In this way $N_R=N_{X_f}$. Defining V_R and V_{X_f} by the equalities $U(R)=e(Y)V_R$ and $U(X_f)=e(X)V_{X_f}$, $V_R/V_{X_f} \to 1$ as all $N_\alpha\to\infty$, because $\rho(X)=\rho(Y)$. On the other hand,

from the convergence (10) it follows that the interaction terms are of smaller order, $V_R^{-1}I(X_f, X\backslash X_f)$ and $V_R^{-1}I(R, X\backslash X_f)$ tend to zero. This ends the proof of the proposition.

The proposition implies the assertion (ii) of the theorem, because any ground state configuration Y of density $\rho(Y) = \rho(X)$, described in (i), has an energy density $e(Y) = \epsilon(\rho(X)) < e(X)$.

IV. SUMMARY

In this paper we have described the ground state configurations of pair interactions φ and $\varphi+\psi$, where φ is the inverse Fourier transform of a non-negative function vanishing outside the sphere of radius K_0, and ψ is a non-negative finite-range interaction of range r_0. The GSCs of φ alone could be obtained, as already in Ref. 1, above a threshold density ρ_d, while those of $\varphi+\psi$ in a density interval whose lower boundary is ρ_d and the upper boundary is the close-packing density of hard balls of diameter r_0. Below this density, ψ alone would allow as a GSC any configuration with a nearest-neighbor distance not smaller than r_0; combined with φ, its role is to decrease the degeneracy of the GSCs of φ. This reduced degeneracy is still continuous inside the interval, but at the boundaries $\varphi+\psi$ has a unique GSC, which is, in three dimensions, the bcc lattice at the lower and the fcc lattice at the upper density limit. This transition from a bcc ground state at $\rho=\rho_3$ to an fcc one at $\rho=\sqrt{2}/r_0^3$ is the most interesting finding of the present work.

The method used in Ref. 1 and in this paper cannot be applied to obtain the ground states of φ below ρ_d. The threshold value is a true critical density separating the high-density continuously degenerate region from the low-density region in which the GSC is presumably unique, apart from Euclidean transformations. If $\hat{\varphi}(\mathbf{0}) > 0$, the analytic form of the relation between the density and the chemical potential also changes at ρ_d, see Ref. 1 We expect that at least in a subclass of interactions the unique bcc ground state at ρ_3 survives at lower densities. Similarly, the mathematical method used here is not suitable to obtain the ground states of $\varphi+\psi$ above the upper density limit. Again, this limit seems to be a true critical value, with a continuously degenerate ground state below and, probably, a unique ground state above it. This unique ground state may depend on the details of ψ, but we expect it to be the fcc lattice for a subclass of positive interactions. To clarify these questions, and also the nature of the curious liquidlike ground state between the fcc and bcc phases will be the subject of future research.

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