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Classical Ground States in One Dimension[1]

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We give conditions on an interaction sufficient to guarantee that in one dimension it yield a periodic ground state with one or two particles per unit cell.

KEY WORDS: Ground state; crystal; symmetry.

1. INTRODUCTION

It is remarkable how much has been learned about the solid state without having an intuitive idea why matter exists in a solid phase. Specifically, there is no known mechanism to explain why, at low temperature and/or high pressure, molecules strongly tend to highly symmetric, crystalline configurations. (See Refs. 1–3.)

Aside from helium, where in fact quantum effects prevent the system from solidifying at low pressure, it is expected that one should be able to satisfactorily model the crystal problem with classical particles interacting through phenomenological potentials. The first such models, mostly for molecular-bound systems, appeared in the last few years using one and two dimensions and rather specific interactions.[(4–14)]

Following a recent paper[(15)] we plan to extend this work using the DLR equations[(16–18)] and more general classes of interactions. By using the DLR equations (in fact only their zero temperature limit) we take into account a very wide range of possible boundary conditions while simultaneously avoiding the edge effects that appear in finite particle models. In this framework we give rather general conditions (based heavily on the work of Ventevogel[(5)]) sufficient for one-dimensional models of molecular-

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bound systems to have periodic ground states with one or two particles per unit cell. Lennard-Jones-type two-body potentials, $V(x) = x^{-m} - x^{-n}$, with any chemical potential $\mu \geqslant 0$ (i.e., high pressure), satisfy all our conditions if $m > n \geqslant 3$.

2. NOTATION

We consider models consisting of countably many point particles in one space dimension interacting through a two-body and one-body (chemical) potential. If x and y are two distinct positions in $\mathbb{R}$, the interactions are described by $W(x, y) = V(|x - y|)$, $|x - y|$ denoting the separation of x and y, and $W(x, x) = -\mu$ (independent of x), where $\mu \geqslant 0$ and V satisfies

$$V = V_1 - V_2, \qquad V_j \text{ convex on } (0, \infty), \quad j = 1, 2 \tag{1}$$

$$V_j(x) = o(x^{-2}) \qquad \text{as} \quad x \to \infty, \quad j = 1, 2. \tag{2}$$

$$\begin{aligned} &1/V(x) = o(x) \qquad \text{as} \quad x \searrow 0, \quad \text{and} \\ &\sum_{k \geqslant 1} V(ka) \text{ is negative for some } a > 0 \end{aligned} \tag{3}$$

(Note: it would be easy to accommodate for a hard core.)

By a "configuration" we mean any countable locally finite subset of $\mathbb{R}$. C denotes the set of all configurations, $C^p \subset C$ the subset of periodic configurations, and $C_n^p \subset C^p$ the subset of those with less than or equal to n points per unit cell. Given any interaction W, finite open interval I, and configuration T we define

$$E_I(T, W) = \sum_{\substack{x,y \in T \\ \{x,y\} \cap I \neq \varnothing \\ x \leqslant y}} W(x, y) \quad \text{and} \quad e(T, W) = \liminf_{I \nearrow \mathbb{R}} E_I(T, W)/|I|$$

where $|I|$ denotes the length of I.

A configuration S is said to be a "ground state (for W)" if, for any finite open interval I and configuration T such that $T \cap (\mathbb{R} \backslash I) = S \cap (\mathbb{R} \backslash I)$, it follows that $E_I(S, W) \leqslant E_I(T, W)$. (See Ref. 17.) It is easy to show that a ground state S satisfies $e(S, W) = \inf_{T \in C} e(T, W)$ but that a solution S of this equation need not be a ground state. However there is the following result of Sinai (see p. 36 in Ref. 17).

Theorem 1 (Sinai). If a periodic configuration S satisfies

$$e(S, W) = \inf_{T \in C^p} e(T, W) \tag{4}$$

then S is a ground state.

Proof. Suppose $S \in C^p$, with period c, satisfies (4) and is not a ground state. Then there exists a finite open interval I and a configuration

T such that $T \cap (\mathbb{R}\backslash I) = S \cap (\mathbb{R}\backslash I)$ and $E_I(S, W) - E_I(T, W) \equiv b > 0$. We construct $\tilde{T} \in C^p$ as follows. Let $r > 0$ be the minimal spacing in T [which exists from (3)] and, using (2), let $R > 0$ be such that

$$|V(x)| < br^2/(40x^2) \qquad \text{for} \quad x > R \tag{5}$$

$$R > c + |I| \tag{6}$$

$$R \text{ is an integer multiple of } c \tag{7}$$

Let t be the midpoint of I and $\tilde{T}$ be that configuration of period $4R$ such that $\tilde{T} \cap J = T \cap J$ where J is a half-open interval of length $4R$ centered at t. Now $e(S, W) - e(\tilde{T}, W) \geqslant e(S, W_R) - e(\tilde{T}, W_R) - \Delta e(S, W) - \Delta e(\tilde{T}, W)$ if $\mu_R = \mu$, $V_R = \chi V$, χ the characteristic function of the interval $(0, R)$, and $\Delta e(\tilde{T}, W) \geqslant |e(\tilde{T}, W) - e(\tilde{T}, W_R)|$, $\Delta e(S, W) \geqslant |e(S, W) - e(S, W_R)|$. It is easy to see using (6) that $e(S, W_R) - e(\tilde{T}, W_R) = [E_I(S, W_R) - E_I(T, W_R)]/4R$. Now

$$|E_I(T, W_R) - E_I(T, W)| \leqslant \frac{R}{r} \frac{br^2}{40} 2 \sum_{j \geqslant 0} \frac{1}{(R + jr)^2} < \frac{b}{10}$$

and similarly $|E_I(S, W_R) - E_I(S, W)| < b/10$, so $e(S, W_R) - e(\tilde{T}, W_R) \geqslant b/5R$. Also,

$$|e(\tilde{T}, W) - e(\tilde{T}, W_R)| \leqslant \frac{1}{4R} \frac{4R}{r} \frac{br^2}{40} 2 \sum_{j \geqslant 0} \frac{1}{(R + jr)^2} < \frac{1}{10R}$$

and similarly $|e(S, W) - e(S, W_R)| < 1/10R$, which implies $e(S, W) - e(\tilde{T}, W) > 0$ which contradiction proves the theorem. ■

Note: It is straightforward to generalize the proof to n-dimensional models.

3. MAIN RESULTS

Our objective is to give general conditions on an interaction sufficient to guarantee that there are periodic ground states. *We know from Ref.* 9 *that conditions* (1)–(3) *are not sufficient*. Consider the conditions

$$V \text{ is monotone increasing on } (v, \infty) \text{ for some } v < \infty \tag{8}$$

$$P(y) \equiv V(y) - \sum_{k \geqslant 2} V_2(ky) \qquad \text{is convex on } (0, v) \tag{9}$$

$$\begin{aligned} Q(x, y, z) \equiv{} & V(x) + V(x + y) + V(x + y + z) \\ & - \sum_{k \geqslant 4}^{(e)} V_2(k(x + y)/2) - \sum_{k \geqslant 4}^{(o)} V_2(x + (k - 1)(y + z)/2) \\ & \text{is convex in the vector variable } (x, y, z)\text{, where each} \\ & \text{component of } (x, y, z) \text{ is restricted to } (0, v) \end{aligned} \tag{10}$$

In (10) and below $\sum^{(e)}$ (resp. $\sum^{(o)}$) refers to summation restricted to even (resp. odd) values of the index.

Theorem 2 (Ventevogel[4]). If V satisfies (8) and (9) there is a solution S of (4) in C_1^p.

Proof. First we note that if T is any periodic configuration and if any of the nearest-neighbor separations in T are larger than v then by (8) it follows that $e(T, W)$ would not increase if all such separations are reduced to v. Now let T be any periodic configuration with period L whose separations are all less than or equal to v; specifically assume $T = \{x_j\}$, $0 < x_{j+1} - x_j \leqslant v$, $x_{j+N} = x_j + L$, $-\infty < j < \infty$. Define $z_j = x_{j+1} - x_j$, so that $0 < z_j \leqslant v$ and

$$\sum_{n=1}^{N} z_{n+j} = L \qquad \text{for all } j \tag{11}$$

Without loss of generality we assume N is even; L need not be the smallest period of T.

Lemma 1. $(1/N)\sum_{n=1}^{N} V_1(\sum_{m=1}^{k} z_{n+m}) \geqslant V_1(kL/N)$, $1 \leqslant k < \infty$.

Proof. Immediate from the convexity of V_1 and the periodicity of T. ■

Lemma 2. $\sum_{n=1}^{N} V_2(\sum_{m=1}^{k} z_{n+m}) \leqslant \sum_{n=1}^{N} V_2(kz_{n+j})$, $1 \leqslant k < \infty$, $-\infty < j < \infty$.

Proof. By convexity $(1/k)\sum_{m=1}^{k} V_2(kz_{n+m}) \geqslant V_2((k/k)\sum_{m=1}^{k} z_{n+m})$, so $\sum_{n=1}^{N} V_2(\sum_{m=1}^{k} z_{n+m}) \leqslant (1/k)\sum_{n=1}^{N}\sum_{m=1}^{k} V_2(kz_{n+m})$. But from (11), $\sum_{m=1}^{k}\sum_{n=1}^{N} V_2(kz_{n+m}) = k\sum_{n=1}^{N} V_2(kz_{n+j})$ for any j, which proves the lemma. ■

Using Lemmas 1 and 2,

$$\begin{aligned} e(T, W) &= (1/L)\sum_{n=1}^{N}\sum_{k\geqslant 1} V\left(\sum_{m=1}^{k} z_{n+m}\right) - \mu N/L \\ &= (1/L)\sum_{n=1}^{N} V_1(z_{n+1}) + (1/L)\sum_{n=1}^{N}\sum_{k\geqslant 2} V_1\left(\sum_{m=1}^{k} z_{n+m}\right) \\ &\quad - (1/L)\sum_{n=1}^{N}\sum_{k\geqslant 1} V_2\left(\sum_{m=1}^{k} z_{n+m}\right) - \mu N/L \end{aligned}$$

$$\geqslant (1/L)\sum_{n=1}^{N} V_1(z_{n+1}) + (N/L)\sum_{k\geqslant 2} V_1(kL/N)$$

$$-(1/L)\sum_{n=1}^{N}\sum_{k\geqslant 1} V_2(kz_{n+1}) - \mu N/L$$

$$\geqslant (1/L)\sum_{n=1}^{N} P(z_{n+1}) + (N/L)\sum_{k\geqslant 2} V_1(kL/N) - \mu N/L$$

where $P(y) = V(y) - \sum_{k\geqslant 2} V_2(ky)$. Then from (9)

$$e(T,W) \geqslant (N/L)\left[P(L/N) + \sum_{k\geqslant 2} V_1(kL/N) - \mu\right]$$

$$\geqslant (N/L)\left[\sum_{k\geqslant 1} V(kL/N) - \mu\right]$$

which proves the result as the right-hand side is the energy density of a configuration in C_1^p and using (1)–(3) this quantity assumes a minimum at some S in C_1^p. ■

Example. Let $V(x) = x^{-m} - x^{-n}$, $m > n > 2$. We want conditions on m and n such that V satisfies (1)–(3), (8), and (9). Now $V''(x) > 0$ for $0 < x < x_I$, where x_I is the solution of $m(m+1)x^{-m} = n(n+1)x^{-n}$, and V is monotone on (x_C, ∞), where x_C is the solution of $mx^{-m} = nx^{-n}$. Then we define $V_2 = V_1 - V$, where

$$V_1(x) = \begin{cases} ax + b + V(x), & 0 < x \leqslant x_I \\ 0, & x_I < x \end{cases}$$

and $a = -V'(x_I)$, $b = -ax_I - V(x_I)$. Note that $V_1''(x_I) = V_1'(x_I) = V_1(x_I) = 0$, $V_1(x) \geqslant 0$ for all x, and V_1, V_2 are convex. It is easy to see that on $(0, x_I)$

$$P''(x) \geqslant \sum_{k\geqslant 1} k^2 V''(kx) > \sum_{k\geqslant 1} (nx^{-n}/x^2)\left[(m+1)k^{-m} - (n+1)k^{-n}\right]$$

and so P is convex on $(0, x_C)$ if

$$(m+1)\zeta(m) > (n+1)\zeta(n) \tag{12}$$

where $\zeta(y) \equiv \sum_{k\geqslant 1} k^{-y}$. Condition (12) is quite mild. For instance it is easy to check that it is satisfied if $m > n \geqslant 3$.

Theorem 3. If V satisfies (8) and (10) there is a solution S of (4) in C_2^p.

Proof. We use the same notation as in the last proof. Thus

$$
\begin{aligned}
e(T,W) &= (1/L)\sum_{n=1}^{N}\sum_{k\geqslant 1} V\left(\sum_{m=1}^{k} z_{n+m}\right) - \mu N/L \\
&= (1/L)\sum_{n=1}^{N} V(z_{n+1}) + (1/L)\sum_{n=1}^{N} V(z_{n+1}+z_{n+2}) \\
&\quad + (1/L)\sum_{n=1}^{N} V(z_{n+1}+z_{n+2}+z_{n+3}) \\
&\quad + (1/L)\sum_{n=1}^{N}\sum_{k\geqslant 4}{}^{(\mathrm{e})} V_1\left(\sum_{m=1}^{k} z_{n+m}\right) \\
&\quad + (1/L)\sum_{k\geqslant 4}{}^{(\mathrm{o})}\left\{\sum_{n=1}^{N}{}^{(\mathrm{o})} V_1\left(\sum_{m=1}^{k} z_{n+m}\right) + \sum_{n=1}^{N}{}^{(\mathrm{e})} V_1\left(\sum_{m=1}^{k} z_{n+m}\right)\right\} \\
&\quad - (1/L)\sum_{n=1}^{N}\sum_{k\geqslant 4}{}^{(\mathrm{e})} V_2\left(\sum_{m=1}^{k} z_{n+m}\right) \\
&\quad - (1/L)\sum_{k\geqslant 4}{}^{(\mathrm{o})}\left\{\sum_{n=1}^{N}{}^{(\mathrm{o})} V_2\left(\sum_{m=1}^{k} z_{n+m}\right)\right. \\
&\qquad\qquad \left. + \sum_{n=1}^{N}{}^{(\mathrm{e})} V_2\left(\sum_{m=1}^{k} z_{n+m}\right)\right\} - \mu N/L
\end{aligned}
\tag{13}
$$

For even k,

$$
\begin{aligned}
&\sum_{n=1}^{N} V_2[k(z_{n+1}+z_{n+2})/2] \\
&\quad = [1/(k/2)]\sum_{m=1}^{k}{}^{(\mathrm{o})}\sum_{n=1}^{N} V_2[k(z_{n+m}+z_{n+m+1})/2] \\
&\quad \geqslant \sum_{n=1}^{N} V_2\left[\sum_{m=1}^{k}{}^{(\mathrm{o})}(z_{n+m}+z_{n+m+1})\right]
\end{aligned}
\tag{14}
$$

For odd k,

$$
\begin{aligned}
&\sum_{n=1}^{N}{}^{(\mathrm{o})} V_2[z_{n+1}+(k-1)(z_{n+2}+z_{n+3})/2] \\
&\quad = \{1/[(k-1)/2]\}\sum_{m=1}^{k}{}^{(\mathrm{e})}\sum_{n=1}^{N}{}^{(\mathrm{o})} V_2[z_{n+1}+(k-1)(z_{n+m}+z_{n+m+1})/2] \\
&\quad \geqslant \sum_{n=1}^{N}{}^{(\mathrm{o})} V_2\left(\sum_{m=1}^{k} z_{n+m}\right)
\end{aligned}
\tag{15}
$$

Similarly, for odd k

$$\sum_{n=1}^{N}{}^{(e)} V_2[z_{n+1} + (k-1)(z_{n+2} + z_{n+3})/2] \geqslant \sum_{n=1}^{N}{}^{(e)} V_2\left(\sum_{m=1}^{k} z_{n+m}\right) \quad (16)$$

Using (14)–(16), (13) becomes

$$\begin{aligned}
e(T,W)& \\
\geqslant{}& (1/L)\sum_{n=1}^{N} V(z_{n+1}) + (1/L)\sum_{n=1}^{N} V(z_{n+1}+z_{n+2}) \\
&+ (1/L)\sum_{n=1}^{N} V(z_{n+1}+z_{n+2}+z_{n+3}) + (1/L)\sum_{n=1}^{N}\sum_{k\geqslant 4}{}^{(e)} V_1\left(\sum_{m=1}^{k} z_{n+m}\right) \\
&+ (1/L)\sum_{k\geqslant 4}{}^{(o)}\left[\sum_{n=1}^{N}{}^{(o)} V_1\left(\sum_{m=1}^{k} z_{n+m}\right) + \sum_{n=1}^{N}{}^{(e)} V_1\left(\sum_{m=1}^{k} z_{n+m}\right)\right] \\
&- (1/L)\sum_{n=1}^{N}\sum_{k\geqslant 4}{}^{(e)} V_2[k(z_{n+1}+z_{n+2})/2] \\
&- (1/L)\sum_{k\geqslant 4}{}^{(o)}\left\{\sum_{n=1}^{N}{}^{(o)} V_2[z_{n+1}+(k-1)(z_{n+2}+z_{n+3})/2]\right. \\
&\qquad\left. + \sum_{n=1}^{N}{}^{(e)} V_2[z_{n+1}+(k-1)(z_{n+2}+z_{n+3})/2]\right\} \\
&- \mu N/L \\
\geqslant{}& (N/L)\Bigg((1/N)\sum_{n=1}^{N}{}^{(e)}\Bigg\{V(z_{n+1}) + V(z_{n+1}+z_{n+2}) \\
&\qquad + V(z_{n+1}+z_{n+2}+z_{n+3}) \\
&\qquad + \sum_{k\geqslant 4}{}^{(e)} V_1\left(\sum_{m=1}^{k} z_{n+m}\right) + \sum_{k\geqslant 4}{}^{(o)} V_1\left(\sum_{m=1}^{k} z_{n+m}\right) \\
&\qquad - \sum_{k\geqslant 4}{}^{(e)} V_2[k(z_{n+1}+z_{n+2})/2] \\
&\qquad - \sum_{k\geqslant 4}{}^{(o)} V_2[z_{n+1}+(k-1)(z_{n+2}+z_{n+3})/2]\Bigg\}\Bigg) \\
&+ (N/L)\left\{(1/N)\sum_{n=1}^{N}{}^{(o)}\{[\text{same}]\}\right\} - \mu N/L
\end{aligned}$$

Using (10), the convexity of V_1 and the notation $\langle z\rangle_o = (2/N)\sum_{n=1}^{N(o)} z_n$, $\langle z\rangle_e = (2/N)\sum_{n=1}^{N(e)} z_n$,

$$
\begin{aligned}
e(T, W)& \\
\geqslant [N/(2L)]\Big\{ & V(\langle z\rangle_o) + V(\langle z\rangle_e + \langle z\rangle_o) + V(\langle z\rangle_e + 2\langle z\rangle_o) \\
&+ \sum_{k\geqslant 4}^{(e)} V_1[k(\langle z\rangle_e + \langle z\rangle_o)/2] \\
&+ \sum_{k\geqslant 4}^{(o)} V_1[\langle z\rangle_o + (k-1)(\langle z\rangle_e + \langle z\rangle_o)/2] \\
&- \sum_{k\geqslant 4}^{(e)} V_2[k(\langle z\rangle_e + \langle z\rangle_o)/2] \\
&- \sum_{k\geqslant 4}^{(o)} V_2[\langle z\rangle_o + (k-1)(\langle z\rangle_e + \langle z\rangle_o)/2]\Big\} \\
+ [N/(2L)]&[\text{same with “even” and “odd” subscripts interchanged}] \\
- \mu N/L& \\
\geqslant (N/L)\Big\{ & \sum_{k\geqslant 1}^{(e)} V[k(\langle z\rangle_e + \langle z\rangle_o)/2] \\
&+ (1/2)\sum_{k\geqslant 1}^{(o)} V[\langle z\rangle_o + (k-1)(\langle z\rangle_e + \langle z\rangle_o)/2] \\
&+ (1/2)\sum_{k\geqslant 1}^{(o)} V[\langle z\rangle_e + (k-1)(\langle z\rangle_e + \langle z\rangle_o)/2] - \mu\Big\}
\end{aligned}
$$

which proves the theorem since the right-hand side is the energy density of a configuration in C_2^p which, using (1)–(3), assumes a minimum at some S in C_2^p. ■

Remark. The above consists, with minor adjustments and generalizations, of the application of a result of Sinai to one of Ventevogel, to the effect of enabling the latter to include general nonperiodic configurations in the energy-density minimization scheme.

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