

THE BRIDGED CROSS-POLYTOPE FRAMEWORK: UNIT-SPRING ELASTIC CONSTANTS IN EVERY DIMENSION AND AN EXACT MOTION FROM THE CaB_6 BORON NET TO FACE-CENTRED CUBIC PACKING

AHRAZ ARIFUDDIN

ABSTRACT. Place a ball at the incentre of each of the $2n$ pyramids that join the centre of an n -cube to its facets. The balls form regular cross-polytopes, one per cell of the cubic lattice, and neighbouring cross-polytopes touch through one bar per axis. In three dimensions this is the boron net of CaB_6 (RCSR *cab*). We prove two results about this bridged cross-polytope framework. First, with unit springs on all bars, every shear modulus vanishes, $C_{11}/C_{12} = (n-1)^2$, and the Poisson ratio for uniaxial stress along a cube axis is $\nu_{100} = 1/(n^2 - n - 1)$, for every $n \geq 3$. Second, in three dimensions there is an explicit motion, rational in a parameter s over $\mathbb{Q}(\sqrt{2})$, that keeps every bar length, keeps the octahedra in a fixed orientation while the lattice deforms, raises the packing fraction strictly from 0.2233 to $\pi/\sqrt{18}$, and ends in face-centred cubic packing. No two balls overlap at any parameter value; we give a written proof that uses the monoclinic symmetry of the path and a bound on the deformed lattice, and an independent exact certificate. The zero-mode and self-stress counts $n(n-1)/2$ and $n(n-3)/2$ per cell, on which the elastic proof rests, are recorded as lemmas: the same periodic graph appears in Borcea and Streinu, and the counts follow from standard periodic-rigidity arguments. As secondary results we record a radius-ratio identity for the incentre construction, with its exact hypotheses and counterexamples, and the maximal hard-sphere packing fraction $(\pi/6)(30\sqrt{2}-41)$ of the CaB_6 structure type. Every number is reproduced by scripts in a public repository.

Version 2. Supersedes v1 (doi:10.5281/zenodo.23322080), whose novelty claims for the rigidity counts are corrected here.

1. INTRODUCTION

Draw a square and its diagonals, mark the incentre of each of the four triangles, and repeat the square over the plane. A ball of the inradius at each incentre touches its two neighbours across the diagonals and one ball of the next square across the shared side. The same holds in every dimension. If an n -cube of side 2 is cut into the $2n$ pyramids that join its centre to its facets, the incentre of each pyramid lies on an axis at distance $c = 2 - \sqrt{2}$ from the centre and has inradius $R = \sqrt{2} - 1$. Balls of radius R at these $2n$ points touch along all edges of the cross-polytope they span and across every facet of the cubic tiling (Fig. 1). The bars between touching balls form a periodic framework: regular cross-polytopes, one per cell, joined by one bridge per axis. We call it the *bridged cross-polytope framework*.

What is known. The triangles of the drawing are fundamental domains of the $[4, 4]$ reflection group, and the orbit of the incentre is the vertex set of the truncated square tiling 4.8.8; in dimension n the incentre is the Wythoff point of $t_{0,1}\{4, 3^{n-2}, 4\}$ [9, 7, 18]. In three dimensions the vertex set, with equal bonds, is the boron net of CaB_6 in the model of Pauling and Weinbaum [33], the RCSR net *cab* [31, 35, 10]. As a framework of rigid octahedra joined by linear bridges it has the Prussian-blue topology, whose rigid unit modes were analysed by Goodwin [16]; Li, Refson and Dove studied the rigid unit modes of the B_6 octahedra in real hexaborides [25].

Borcea and Streinu [4, Section 7] describe the same periodic graph in every dimension: two orbits of regular cross-polytopes under their periodicity lattice, each vertex joined by a bar to a vertex of a neighbouring cross-polytope, with bars twice the cross-polytope edge. In our notation (Section 2) their realization has the dots at $t = \sqrt{2} - 1$ instead of $t = 2 - \sqrt{2}$; the counts below hold for every $t \in (0, 1)$ and so cover it. They give the three-dimensional count (nine degrees of freedom with a variable lattice) and sketch a three-dimensional folding to a folded state; it is not a packing. The periodic rigidity theory we use is standard [3, 26, 34]. We claim none of this.

What we add.

- (1) Theorem 1: the unit-spring elastic tensor of the bridged cross-polytope framework in every dimension $n \geq 3$: all shear moduli vanish, $C_{11}/C_{12} = (n - 1)^2$ and $\nu_{100} = 1/(n^2 - n - 1)$. We did not find these formulas in the sources we read (Section 4). The proof uses a decomposition of the rigidity matrix by the sign-change symmetries of the cross-polytope, which also gives the mode and self-stress counts with explicit bases (Lemmas 2 and 3). We present those counts as lemmas that follow from existing machinery.
- (2) Theorem 2: an exact, continuous, bar-preserving and overlap-free motion from the cab framework to face-centred cubic (fcc) packing, with strictly increasing density. It is a single closed-form curve, rational in its parameter over $\mathbb{Q}(\sqrt{2})$. The octahedra keep their orientation and the lattice deforms, changing volume by a factor of 3.3. Non-overlap has a written proof (Section 5) and an exact computer certificate.
- (3) Secondary results: a radius-ratio identity for the incentre construction (Theorem 3), and the maximal packing fraction of the CaB₆ structure type (Theorem 4), with supporting results on numerical paths to hcp and fcc and on the planar and cubic-restricted motions (Section 6).

Changes from v1. The title and the headline are new. Version 1 presented the zero-mode and self-stress counts as its main result and stated that the n -dimensional closed forms were not found in the literature. That framing is withdrawn: Borcea and Streinu [4, Section 7] describe the same graph in every dimension, and the counts follow from standard arguments; they are now Lemmas 2–3. The elastic constants, which v1 also proved, are now the first headline result. The exact motion to fcc (Section 5) is new in v2, as are the summaries of the numerical paths and exact end states. The CaB₆ attainment step, checked over a finite block of cells in v1, is now proved for all pairs, and the possible earlier statement of the peak location by Travesset is noted. Script paths and references were corrected, and references on periodic rigidity, sphere-packing deformations and the ReO₃ analogue were added.

2. THE FRAMEWORK

Let $Q_n = [-1, 1]^n$ and let $\mathbf{e}_1, \dots, \mathbf{e}_n$ be the standard basis. The pyramid over the facet $x_i = 1$ is $\{x \in Q_n : x_i \geq |x_j| \ \forall j\}$, with base $x_i = 1$ and walls $x_i = \pm x_j$. A point $t\mathbf{e}_i$ has distance $1 - t$ to the base and $t/\sqrt{2}$ to every wall, so the incentre is $c\mathbf{e}_i$ with

$$c = 2 - \sqrt{2}, \quad R = 1 - c = \sqrt{2} - 1, \quad c\sqrt{2} = 2R.$$

The dots are $p_i^s = sc\mathbf{e}_i$ for $i = 1, \dots, n$ and $s \in \{+1, -1\}$. Two dots on different axes are at distance $c\sqrt{2} = 2R$, and p_i^+ is at distance $2 - 2c = 2R$ from the dot $p_i^- + 2\mathbf{e}_i$ of the next cell. All other distances are larger.

Definition 1. The *bridged cross-polytope framework* $\mathcal{F}_n$ has the dots $p_i^s + 2z$ ($z \in \mathbb{Z}^n$) as joints and a bar between every pair of touching balls: the $2n(n - 1)$ *intra bars* $\{p_i^s, p_j^t\}$, $i < j$, of each cell (the edges of the cross-polytope), and the n *bridges* $X_i = \{p_i^+, p_i^- + 2\mathbf{e}_i\}$ per cell. Every bar has length $2R$. More generally, $\mathcal{F}_n(t)$ has the same graph with dots at $\pm t\mathbf{e}_i$, $0 < t < 1$.

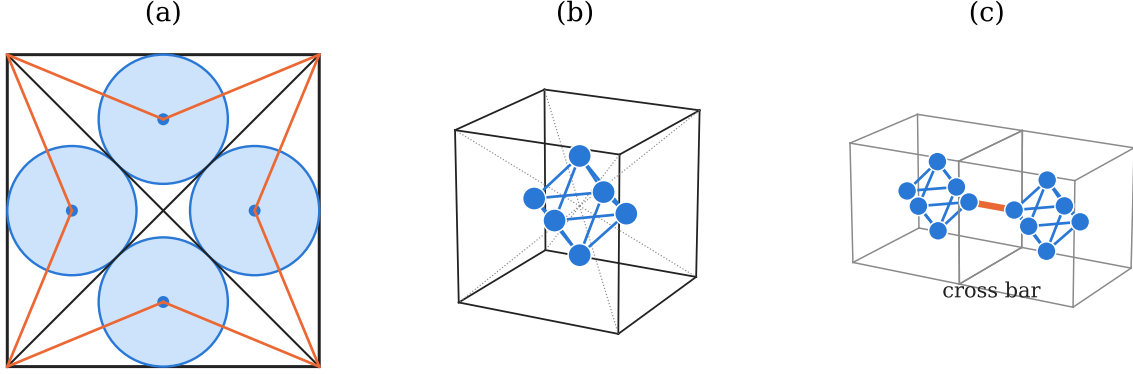


FIGURE 1. (a) The planar construction: incentres of the four triangles cut by the diagonals, with balls of the inradius and lines to the corners. (b) In three dimensions the six incentres of the centre-to-face pyramids form an octahedron of edge $2R$. (c) Two cells of the framework: the cross-polytope bars inside each cell and one bridge between cells.

Per cell there are $2n$ joints, hence $2n^2$ degrees of freedom, and $2n^2 - n$ bars; each ball touches $2n - 1$ others. For Bloch displacements $\mathbf{u}(p + 2z) = \mathbf{u}(p) e^{2iq \cdot z}$ write $z_i = e^{2iq_i}$. The rigidity matrix $R(q)$ has one row per bar; the row of a bar from joint a to joint b with unit direction $\hat{d}$ is $\mathbf{u} \mapsto \hat{d} \cdot (\mathbf{u}_b - \mathbf{u}_a)$, with $\mathbf{u}_b$ carrying the phase of its cell. A *zero mode* is a vector in $\ker R(q)$ and a *self-stress* a vector in $\ker R(q)^*$. By rank-nullity, the number of zero modes minus the number of self-stresses is $2n^2 - (2n^2 - n) = n$ at every q , the periodic Maxwell–Calladine count [27, 5, 34].

3. ZERO MODES AND SELF-STRESSES

Fix one cell. For displacements $\mathbf{u}_i^s = \mathbf{u}(p_i^s)$ write $\mathbf{a}_i = \frac{1}{2}(\mathbf{u}_i^+ + \mathbf{u}_i^-)$ and $\mathbf{b}_i = \frac{1}{2}(\mathbf{u}_i^+ - \mathbf{u}_i^-)$, and denote the k -th component of a vector by a superscript. For $i < j$ define

$$\alpha_{ij} = a_i^i - a_j^i, \quad \beta_{ij} = a_j^j - a_i^j, \quad \kappa_{ij} = b_i^i + b_j^j, \quad \sigma_{ij} = b_i^j + b_j^i.$$

Lemma 1. *Under a homogeneous strain ε plus displacements $\mathbf{u}$, the first-order extension of the intra bar from p_j^t to p_i^s is*

$$(1) \quad \delta_{ij}^{st} = \frac{1}{\sqrt{2}} \left[c(\varepsilon_{ii} + \varepsilon_{jj}) + \kappa_{ij} + s\alpha_{ij} - t\beta_{ij} - st(2c\varepsilon_{ij} + \sigma_{ij}) \right].$$

For a one-cell-periodic displacement the extension of the bridge X_i is $2R\varepsilon_{ii} - 2b_i^i$; for a Bloch displacement with $\varepsilon = 0$ it is $\mathbf{e}_i \cdot (z_i \mathbf{u}_i^- - \mathbf{u}_i^+)$.

Proof. The bar vector is $\ell = c(\mathbf{s}\mathbf{e}_i - \mathbf{t}\mathbf{e}_j)$, with unit vector $\ell/(c\sqrt{2})$, and $\delta = \hat{\ell} \cdot (\varepsilon\ell + \mathbf{u}_i^s - \mathbf{u}_j^t)$. Expand with $\mathbf{u}_i^s = \mathbf{a}_i + \mathbf{s}\mathbf{b}_i$ and $s^2 = t^2 = 1$. For X_i the bar vector is $2R\mathbf{e}_i$ and the displacement difference is $-2\mathbf{b}_i$ in the periodic case. $\square$

The functions $1, s, t, st$ on $\{\pm 1\}^2$ are orthogonal. So the four bars between axes i and j impose the four scalar conditions $\kappa_{ij} = \alpha_{ij} = \beta_{ij} = \sigma_{ij} = 0$ when $\varepsilon = 0$, and

$$(2) \quad \frac{1}{2} \sum_{s,t} (\delta_{ij}^{st})^2 = (c(\varepsilon_{ii} + \varepsilon_{jj}) + \kappa_{ij})^2 + \alpha_{ij}^2 + \beta_{ij}^2 + (2c\varepsilon_{ij} + \sigma_{ij})^2.$$

The linear problem splits into independent systems: one in the n numbers b_i^i (through κ), one in the n^2 entries of the $\mathbf{a}_i$ (through α, β), and one in the $n(n-1)$ entries $b_i^j, i \neq j$ (through σ).

Lemma 2 (cross-polytope). *Let $n \geq 3$. The cross-polytope (the intra bars of one cell) is infinitesimally rigid in $\mathbb{R}^n$ and has exactly $n(n-3)/2$ independent self-stresses. A basis: tension w_{ij} on all four bars $\{p_i^\pm, p_j^\pm\}$, where $w = (w_{ij})_{i < j}$ satisfies $\sum_{j \neq i} w_{ij} = 0$ for every i .*

Proof. The conditions $\alpha_{ij} = \beta_{ij} = 0$ say that for each k all a_j^k equal a_k^k , so $\mathbf{a}_j = \mathbf{v}$ for all j ; the map $\mathbf{a} \mapsto (\alpha, \beta)$ from $\mathbb{R}^{n^2}$ to $\mathbb{R}^{n(n-1)}$ has an n -dimensional kernel and is onto. Each σ_{ij} involves b_i^j, b_j^i only, so these $\binom{n}{2}$ conditions are independent and force the off-diagonal part of $B = (b_i^j)$ to be antisymmetric. The conditions $b_i^i + b_j^j = 0$ form the system $x_i + x_j = 0$ on the edges of K_n ; for $n \geq 3$ a triangle forces $x = 0$. Its matrix, the unsigned incidence matrix of K_n , has rank n , and its left kernel (edge weights with $\sum_{j \neq i} w_{ij} = 0$ at each vertex) has dimension $n(n-3)/2$. The kernel of the whole system is therefore $\mathbf{u}_i^s = \mathbf{v} + \Omega p_i^s$ with Ω antisymmetric, the trivial motions, and the number of self-stresses is $2n(n-1) - (2n^2 - n(n+1)/2) = n(n-3)/2$. Expanding a stress on the four bars of a pair in the characters $1, s, t, st$, the s, t and st parts must vanish because the $\mathbf{a}$ - and σ -systems have no relations, and the character-1 parts w_{ij} must satisfy $\sum_{j \neq i} w_{ij} = 0$. $\square$

Lemma 3 (periodic counts). *Let $n \geq 3$. At a wavevector with no $q_i \in \pi\mathbb{Z}$, $\mathcal{F}_n(t)$ has exactly $n(n-1)/2$ zero modes per cell, the infinitesimal rotations of each cross-polytope with the common Bloch phase, and exactly $n(n-3)/2$ self-stresses, those of Lemma 2 with zero tension on the bridges. If exactly k of the q_i lie in $\pi\mathbb{Z}$ there are $n(n-1)/2 + k$ zero modes and $n(n-3)/2 + k$ self-stresses. At $q = 0$ there are $n(n+1)/2$ zero modes and $n(n-1)/2$ self-stresses: for every $w \in \mathbb{R}^{\binom{n}{2}}$, tension w_{ij} on the four bars $\{p_i^\pm, p_j^\pm\}$ and $\sqrt{2} \sum_{j \neq i} w_{ij}$ on X_i .*

Proof. Intra rows carry no phase, so a zero mode restricts on each cell to $\mathbf{u}_i^s = \mathbf{v} + \Omega p_i^s$ with complex $\mathbf{v}, \Omega$. Since $\mathbf{e}_i \cdot \Omega \mathbf{e}_i = 0$, Lemma 1 turns the bridge X_i into $(z_i - 1)v^i = 0$: rotations survive at every phase and each $z_i = 1$ frees one translation. The self-stress counts follow from rank-nullity, and the stated stresses balance every joint. $\square$

Remark 1 (credit and scope). These counts use only the internal rigidity of the cross-polytope, the fact that a rotation moves each bridge end transversally, and rank-nullity; they are routine applications of the phase-periodic rigidity matrix [34] and of the rigid-unit analysis of linearly bridged frameworks [16]. We record them because the explicit bases are used in Section 4. They use only bar directions, so they hold for $\mathcal{F}_n(t)$ for every $t \in (0, 1)$, including the realization $t = \sqrt{2} - 1$ of [4, Section 7]. With a variable lattice the first-order count of the one-cell framework in three dimensions is 6; for a periodicity lattice with b body orbits the conditional Maxwell count is $(b+1)n(n-1)/2$, which gives the nine of [4] for $b = 2, n = 3$. For $n = 2$ the square has one internal flex, and the counts are 2 and 0 at generic q , 3 and 1 at $q = 0$. The numerical check (Section 4) confirms all counts for $n = 2, \dots, 8$.

4. UNIT-SPRING ELASTIC CONSTANTS IN EVERY DIMENSION

Theorem 1. *Let $n \geq 3$. Give every bar of $\mathcal{F}_n$ unit spring constant, so that a bar extended by δ stores energy $\delta^2/2$, impose a homogeneous strain ε and relax all joints. The energy per unit volume is*

$$(3) \quad W(\varepsilon) = \frac{1}{2^n} \left[\frac{2(n-1)^2}{n^2} \sum_i \varepsilon_{ii}^2 + \frac{2}{n^2} \sum_{i \neq j} \varepsilon_{ii} \varepsilon_{jj} \right],$$

independent of the off-diagonal strains. With $W = \frac{1}{2}C_{ijkl}\varepsilon_{ij}\varepsilon_{kl}$,

$$C_{11} = \frac{4(n-1)^2}{n^2 2^n}, \quad C_{12} = \frac{4}{n^2 2^n}, \quad \frac{C_{11}}{C_{12}} = (n-1)^2,$$

every component of C involving a shear strain vanishes, and the Poisson ratio for uniaxial stress along a cube axis is

$$\nu_{100} = \frac{C_{12}}{C_{11} + (n-2)C_{12}} = \frac{1}{n^2 - n - 1}.$$

The values of ν_{100} are $1/5, 1/11, 1/19, 1/29, 1/41$ for $n = 3, \dots, 7$ (Fig. 2).

Proof. A homogeneous strain stretches the bars of every cell identically. In a Bloch decomposition of the relaxation over any periodic supercell only the $q = 0$ component couples linearly to ε ; the others add non-negative energy and are optimally zero. So it suffices to relax over one-cell-periodic displacements. By Lemma 1 and (2) the energy per cell is

$$\mathcal{E} = \sum_{i < j} \left[(c(\varepsilon_{ii} + \varepsilon_{jj}) + \kappa_{ij})^2 + \alpha_{ij}^2 + \beta_{ij}^2 + (2c\varepsilon_{ij} + \sigma_{ij})^2 \right] + 2 \sum_i (R\varepsilon_{ii} - b_i^i)^2.$$

The variables $\mathbf{a}$ appear only in α, β ; take $\mathbf{a} = 0$. The off-diagonal b_i^j appear only in σ_{ij} , which can be chosen freely; take $\sigma_{ij} = -2c\varepsilon_{ij}$. This removes every off-diagonal strain, so all shear moduli vanish. (Each cross-polytope stays undeformed; shear is taken up by first-order rotations.)

With $e_i = \varepsilon_{ii}$, $x_i = b_i^i$ and $y_i = x_i + c e_i$, and using $c + R = 1$,

$$\mathcal{E} = \sum_{i < j} (y_i + y_j)^2 + 2 \sum_i (e_i - y_i)^2.$$

The Hessian in y is $2(nI + J)$, with J the all-ones matrix, which is positive definite. Stationarity gives $ny_k + \sum_j y_j = 2e_k$, hence $\sum_j y_j = \frac{1}{n} \sum_j e_j$ and $y_k = \frac{1}{n}(2e_k - \frac{1}{n} \sum_j e_j)$. The minimum of $y^T M y - 2(2e) \cdot y + 2|e|^2$ is $2|e|^2 - 2e \cdot y$, which evaluates to

$$\mathcal{E}_{\min} = \frac{2(n-2)}{n} \sum_i e_i^2 + \frac{2}{n^2} \left(\sum_i e_i \right)^2 = \frac{2(n-1)^2}{n^2} \sum_i e_i^2 + \frac{2}{n^2} \sum_{i \neq j} e_i e_j.$$

Dividing by the cell volume 2^n gives (3). For uniaxial stress along $\mathbf{e}_1$, $\partial W / \partial e_j = 0$ ($j \geq 2$) reads $C_{12}e_1 + (C_{11} + (n-2)C_{12})e_\perp = 0$, and $C_{11} + (n-2)C_{12} = (4/n^2 2^n)((n-1)^2 + n-2)$ gives $\nu_{100} = 1/(n^2 - n - 1)$. $\square$

Remark 2. (1) The proof does not use $n \geq 3$, so (3) also holds for $n = 2$: $C_{11} = C_{12} = 1/4$ and only the bulk modulus is non-zero. (2) For $\mathcal{F}_n(t)$ with unit springs on bars of unequal lengths the same computation applies with $t + (1-t) = 1$ in place of $c + R = 1$, and the formula is unchanged; the incentre $t = c$ is the unique t at which all bars have the same length, so that “unit springs” means “identical bars”. (3) The tensor is only positive semi-definite. The model has no angular stiffness or prestress, and ν_{100} is the response to stress along a cube axis, not an isotropic Poisson ratio or a property of a real compound.

Prior art and check. The formulas follow from minimizing spring energy; rigid-body kinematics alone does not give finite C_{11} or C_{12} . We did not find $C_{11}/C_{12} = (n-1)^2$ or $\nu_{100} = 1/(n^2 - n - 1)$ in Borcea and Streinu [4, Section 7] or in the abstract of Goodwin [16]; this bounded search is not evidence of priority, and the formulas may be immediate to specialists in periodic-framework elasticity. The script `results/rigidity-nd/rigidity_nd.py` builds $R(q)$ and the relaxed elastic tensor from coordinates, without the decomposition, for $n = 2, \dots, 8$. It confirms every count at random q , at $q = 0$ and on the planes $q_1 = \dots = q_k = 0$, that the stated bases span the self-stress spaces and the rotations span the generic zero modes, and the

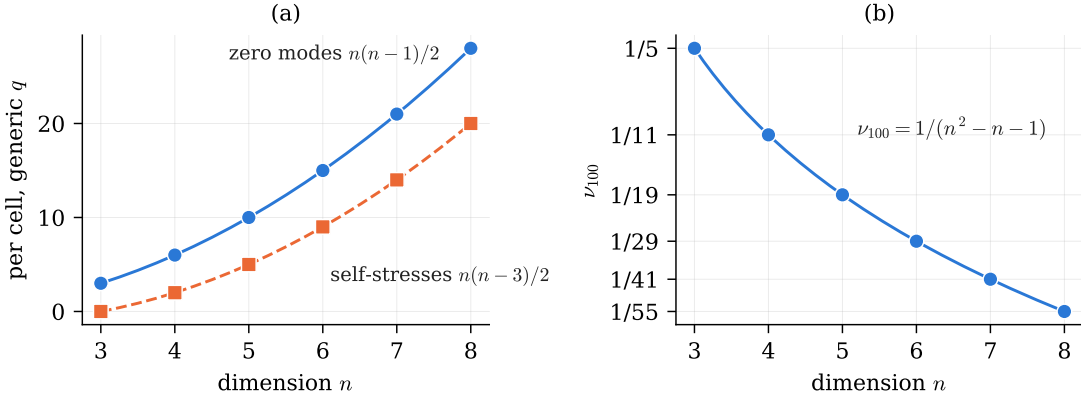


FIGURE 2. (a) Zero modes and self-stresses per cell at a generic wavevector (lines: Lemma 3; markers: rank of the numerically assembled rigidity matrix). (b) Poisson ratio ν_{100} with unit springs (line: Theorem 1; markers: full numerical relaxation).

elastic constants to 10^{-12} with full relaxation, for $c = 2 - \sqrt{2}$ and for $c = 0.3, 0.75$. The script `proof_steps.py` checks (1), (2) and the minimization symbolically for $n = 2, \dots, 8$.

5. AN EXACT MOTION FROM THE CAB FRAMEWORK TO FCC

5.1. The question. Lemma 3 and its variable-lattice analogue describe directions in which $\mathcal{F}_3$ can start to move. They do not say how far it can go. Here balls are joined centre to centre by bars of fixed length and must not overlap. Can the open framework, at packing fraction $\pi R^3 = 0.2233$, be moved continuously to a close packing?

This is not automatic. The natural symmetric motion, the $a^-a^-a^-$ tilt of the octahedra about $[111]$ [15] with the lattice kept cubic, locks at 60° with packing fraction $27\pi\sqrt{2}/256 = 0.4686$ (Section 6). In corner-sharing ReO_3 , by contrast, rotating the octahedra alone takes the anions to hexagonal close packing [30, 22], which is observed under pressure at a rotation of 30° [36]. In the bridged framework the same tilt gives only 0.2637 at 30° . Numerical searches with a free lattice found sampled paths to hcp and fcc, but greedy density ascent from other starting states jams between 0.58 and 0.71 (Section 6). We now give an exact motion.

5.2. The curve. Work in units of $K = 2 - \sqrt{2}$, in which the motif of one cell is

$$P = \{\pm \mathbf{e}_1, \pm \mathbf{e}_2, \pm \mathbf{e}_3\},$$

each ball has radius $1/\sqrt{2}$, and every bar has length $\sqrt{2}$. With row vectors and a lattice matrix L whose rows L_i are the periods, the centres are $p + nL$, $p \in P$, $n \in \mathbb{Z}^3$. The twelve octahedron edges join $\pm \mathbf{e}_i$ to $\pm \mathbf{e}_j$ ($i \neq j$), and the three bridges join $\mathbf{e}_i$ to $-\mathbf{e}_i + L_i$. Multiplying by K and translating by $(1, 1, 1)$ gives the framework $\mathcal{F}_3$ of Section 2, where $KL = 2I$.

Write $\mathbf{b}_i = L_i - 2\mathbf{e}_i$ for the bridge vectors, so $L = 2I + B$ with rows $\mathbf{b}_i$. At the start, $\mathbf{b}_i = \sqrt{2}\mathbf{e}_i$. Let

$$C = \begin{pmatrix} 0 & -1 & -1 \\ 1 & 0 & -1 \\ 1 & -1 & 0 \end{pmatrix}.$$

Its rows C_i satisfy $C_i \cdot \mathbf{e}_i = 0$ and $\|C_i\|^2 = 2$. For $0 \leq s \leq 1$ put

$$(4) \quad t = \frac{2s}{1+s^2}, \quad a = \frac{\sqrt{2}(1-s^2)}{1+s^2}, \quad \mathbf{b}_i(s) = a\mathbf{e}_i + tC_i, \quad L(s) = (2+a)I + tC.$$

Then $a^2 + 2t^2 = 2$. With $\theta = 2 \arctan s$, $\mathbf{b}_i = \sqrt{2}(\cos \theta \mathbf{e}_i + \sin \theta C_i/\sqrt{2})$: each bridge turns through a right angle, at the same rate, in the plane spanned by its initial direction $\mathbf{e}_i$ and its final direction C_i , keeping length $\sqrt{2}$. The motif does not move. The endpoint is

$$L(1) = 2I + C = \begin{pmatrix} 2 & -1 & -1 \\ 1 & 2 & -1 \\ 1 & -1 & 2 \end{pmatrix}.$$

Where C comes from. The integer matrix $L(1)$ is the exact fcc end state of a numerical path in the one-cell framework (Section 6): there the octahedron ends unrotated in its own frame, and the bridges are the rows of C . The curve (4) is the simplest motion that joins the two bridge configurations: each bridge rotates uniformly from $\sqrt{2}\mathbf{e}_i$ to C_i , which is possible with constant length because $C_i \perp \mathbf{e}_i$. That this rotation never makes two balls overlap is the content of Theorem 2. Straight-line interpolation of the bridges would shorten them.

Theorem 2. *For $0 \leq s \leq 1$, the curve (4) is a smooth periodic motion of the three-dimensional bridged cross-polytope framework with the following properties.*

- (a) *Every bar has length $\sqrt{2}$, the lattice is nonsingular, and the octahedra keep their orientation.*
- (b) *No two balls overlap: all distinct centres are at least $\sqrt{2}$ apart. For $0 \leq s < 1$ the only touching pairs are the 15 bars per cell; at $s = 1$ another 21 contacts per cell appear at once, and each ball touches 12 others.*
- (c) *The packing fraction $2\sqrt{2}\pi/\det L(s)$ increases strictly from $2\sqrt{2}\pi/(2+\sqrt{2})^3 = 0.2233$ to $\pi/\sqrt{18}$, and $\det L$ falls from $(2+\sqrt{2})^3$ to 12.*
- (d) *At $s = 1$ the centres form a translate of the fcc lattice.*
- (e) *For $0 < s \leq 1$ the framework has space group $C2/m$, with point group $\{I, -I, m, -m\}$, where m exchanges the second and third coordinates; the balls form two orbits, $\{\pm\mathbf{e}_1\}$ on the mirror and $\{\pm\mathbf{e}_2, \pm\mathbf{e}_3\}$ in general position. At $s = 0$ the space group is $Pm\bar{3}m$.*

The motion is a deformation of the lattice, not a shear alone: the cell volume falls by a factor $(2+\sqrt{2})^3/12 = 3.32$, and the packing fraction rises with it (Fig. 3).

5.3. Proof of (a), (c), (d), (e). The motif is fixed, so the twelve edges keep length $\sqrt{2}$, and $\|\mathbf{b}_i\|^2 = a^2 + 2t^2 = 2$. Nonsingularity follows from the bound below. For (c), with $d = 2 + a$ and $a = \sqrt{2 - 2t^2}$, direct expansion gives $\det L = d^3 + dt^2 + 2t^3$, and for $0 < t < 1$

$$\frac{d}{dt} \det L = \frac{2t}{a}(-16 - 10a + 3t^2 + 3at) < 0,$$

because the bracket is at most $-13 - 7a$. So $\det L$ decreases strictly between any two parameter values, and t increases strictly with s . Each cell holds six balls of volume $(4\pi/3)2^{-3/2}$, which gives the packing fraction. For (d), the rows of $L(1)$ are integer vectors with even coordinate sum and $\det L(1) = 12$, so $\Gamma = \mathbb{Z}^3 L(1)$ has index 6 in $D_3 = \{z \in \mathbb{Z}^3 : \sum z_i \text{ even}\}$, the fcc lattice of covolume 2 [8]. The six motif points have odd coordinate sum and lie in distinct cosets of Γ (by (b) no two centres coincide), so they fill the odd coset of D_3 , an fcc packing with minimum distance $\sqrt{2}$. For (e), m commutes with $L(s)$ (it fixes L_1 and exchanges L_2, L_3), preserves P , and maps bridges to bridges ($\mathbf{b}_1 m = \mathbf{b}_1$, $\mathbf{b}_2 m = \mathbf{b}_3$). Any symmetry maps octahedra to octahedra, so its linear part is a signed permutation preserving the lattice $\mathbb{Z}^3 L(s)$; for $0 < s \leq 1$ only $\pm I$ and $\pm m$ do. The lattice has a basis $L_1, L_2, L_3 = L_2 m$ exchanged by the mirror, so it is centred monoclinic, and the group is $C2/m$.

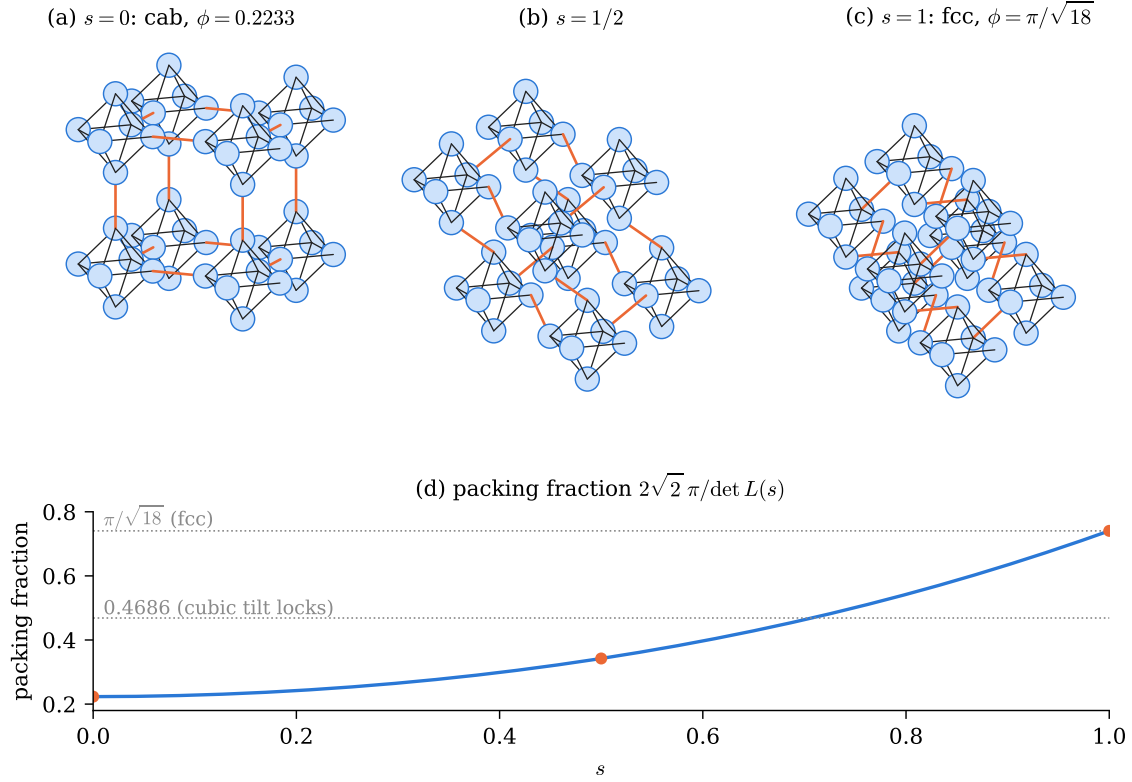


FIGURE 3. The motion of Theorem 2, drawn from the exact formulas. (a)–(c) A block of $2 \times 2 \times 2$ cells at $s = 0, 1/2, 1$, in the same orthographic view; balls are drawn at 0.42 of their radius so that the bars show. Black: octahedron edges; orange: bridges. The octahedra keep their orientation while the lattice deforms. (d) Packing fraction along the motion; the dotted line at 0.4686 is where the cubic-restricted tilt locks, a different path.

5.4. Proof of (b): a reduction to nine one-parameter inequalities. Balls of one octahedron are at least $\sqrt{2}$ apart. For a nonzero integer row n let $w = nL$ be the offset of another octahedron, and let $m_1 \geq m_2 \geq m_3$ be the absolute values of the coordinates of w , sorted. The squared distances between balls of the two octahedra are $\|w + v\|^2$ with $v \in P - P = \{0, \pm 2\mathbf{e}_i, \pm \mathbf{e}_i \pm \mathbf{e}_j\}$. Minimizing $2w \cdot v$ over each type of v , no two of these balls overlap if and only if

$$(5) \quad (A) \|w\|^2 - 4m_1 + 2 \geq 0, \quad (B) \|w\|^2 - 2(m_1 + m_2) \geq 0, \quad (C) \|w\|^2 \geq 2.$$

These conditions are invariant under $n \mapsto -n$ and under the mirror $n \mapsto nm$, which exchanges two coordinates of w .

Lemma 4. *For every $s \in [0, 1]$ the smallest eigenvalue of $L(s)L(s)^T$ is at least $7/3$. Hence octahedra with $\|n\|^2 \geq 5$ have all balls more than $\sqrt{2}$ apart.*

Proof. Using $CC^T = I + J$, one finds $LL^T = (d^2 + t^2)I + t^2J + dtE$, where J is the all-ones matrix and E has $E_{23} = E_{32} = -2$ and zeros elsewhere. In the orthonormal basis $\mathbf{e}_1, (\mathbf{e}_2 + \mathbf{e}_3)/\sqrt{2}, (\mathbf{e}_2 - \mathbf{e}_3)/\sqrt{2}$ it has the eigenvalue $(d + t)^2 \geq 4$ on the last vector, and on the first two the block with diagonal entries $\alpha = d^2 + 2t^2$, $\gamma = d^2 + 3t^2 - 2dt$ and off-diagonal entry $\sqrt{2}t^2$. With $d^2 = 6 + 4a - 2t^2$, $\alpha - \frac{7}{3} = \frac{11}{3} + 4a$ and $\gamma - \frac{7}{3} = \frac{11}{3} - 4t + t^2 + a(4 - 2t) \geq \frac{2}{3}$ for $0 \leq t \leq 1$. So

TABLE 1. The nine classes of nearby octahedra (up to $n \mapsto -n$ and the mirror m), with $d = 2 + a$, $a^2 + 2t^2 = 2$. Slack is the left side of (A) or (B) in (5).

n	$w = nL$	slack in (A)	slack in (B)
$\mathbf{e}_1; \mathbf{e}_2, \mathbf{e}_3$	$(d, -t, -t); (t, d, -t)$	0 (bridge)	$2(1 - t) + 2a$
$(1, 1, 0)$	$(d + t, d - t, -2t)$	$2(1 - t)^2 + 4 + 4a$	$\geq 2(1 - t)^2 + 2 + 4a$
$(1, -1, 0)$	$(d - t, -d - t, 0)$	$2(1 - t)(3 + t) + 4a$	$4 + 4a - 2t^2$
$(0, 1, 1)$	$(2t, d - t, d - t)$	$2(1 - t)(7 - t) + a(8 - 4t)$ or $2(1 - t)^2 + 4 + 4a(1 - t)$	$2(1 - t)(4 - t) + a(6 - 4t)$ or $2(1 - t)^2 + 2 + 4a(1 - t)$
$(0, 1, -1)$	$(0, d + t, -d - t)$	$2(d + t - 1)^2$	$2(d + t)(d + t - 2)$
$(1, 1, 1)$	$(d + 2t, d - 2t, d - 2t)$	$6(t - \frac{4}{3})^2 + \frac{4}{3} + a(8 - 4t)$	$6(t - \frac{2}{3})^2 + \frac{22}{3} + 4a(2 - t)$
$(1, -1, -1)$	$(d - 2t, -d, -d)$	$2(1 - t)(5 + t) + 2 + a(8 - 4t)$	$2(1 - t)(5 + t) + a(8 - 4t)$
$(1, 1, -1)$	$(d, d, -d - 2t)$	$12 + 8a - 2t^2 + 4at$	$10 + 8a - 2t^2 + 4t + 4at$

$(\alpha - \frac{7}{3})(\gamma - \frac{7}{3}) \geq \frac{22}{9} > 2 \geq 2t^4$, and the block minus $\frac{7}{3}I$ is positive semi-definite. If $\|n\|^2 \geq 5$ then $\|nL\|^2 \geq \frac{35}{3} > 6 + 4\sqrt{2} = (2 + \sqrt{2})^2$ (as $289 > 288$), and since $\|v\| \leq 2$ every distance exceeds $\|nL\| - 2 > \sqrt{2}$. $\square$

If $\|n\|^2 = 4$ then $n = \pm 2\mathbf{e}_i$ and $\|nL\|^2 = 4(d^2 + 2t^2) = 4(6 + 4a) \geq 24$. The remaining 26 vectors with $1 \leq \|n\|^2 \leq 3$ form nine classes under sign and mirror. Table 1 lists, for each, the offset $w = dn + t nC$, its squared length, and the slack in (A) and (B), reduced with $a^2 + 2t^2 = 2$. Where the largest coordinate of w depends on s , the slack is given for each candidate. Every entry is visibly non-negative for $0 \leq t \leq 1$, $a \geq 0$, and (C) holds since $\|w\|^2 \geq 6$ throughout. This proves non-overlap for all pairs and all s .

Touching pairs. A slack vanishes identically only for the bridges (class $\mathbf{e}_i$, condition (A)). Otherwise it vanishes only at $t = 1$, $a = 0$, that is $s = 1$, in classes $\mathbf{e}_i$ (B), $(1, -1, 0)$ (A), $(0, 1, 1)$ (A with $m_1 = 2t$, and B with $m_1 + m_2 = d + t$) and $(1, -1, -1)$ (B). These give the 21 new contacts per cell of (b): at $s = 1$ each ball goes from 5 to 12 contacts, all at once. The mirror class of $(1, -1, 0)$ is $(1, 0, -1)$, so at the end each octahedron touches the octahedra at offsets $\pm \mathbf{e}_i$, $\pm(1, -1, 0)$, $\pm(1, 0, -1)$, $\pm(0, 1, 1)$ and $\pm(1, -1, -1)$.

An independent exact certificate. Before the reduction above was found, non-overlap was proved by computer [1]: with the cruder bound $\|nL\| \geq \|n\|$ only the 171 shifts with $\|n\|^2 \leq 11$ remain, giving 3248 conditions $f_{n,v}(s) = (1 + s^2)^2(\|nL(s) + v\|^2 - 2) \geq 0$, each a quartic in s with coefficients in $\mathbb{Q}(\sqrt{2})$. All 16,240 coefficients in the degree-four Bernstein basis are non-negative, decided by exact rational comparisons; since the Bernstein basis functions are non-negative on $[0, 1]$ [11], this proves every inequality on the whole interval. Two separately written implementations agree, and 114 coefficients are zero: five for each of the 18 identically vanishing polynomials (the bars) and one for each of the 24 polynomials that vanish at $s = 1$, matching the contact count above. The written reduction is recorded with a symbolic check of every table entry in `results/fold-continuous-fcc/HAND-PROOF.md`.

5.5. Context. The motion is a statement about an ideal geometric model: bars of fixed length, hard balls, no energy, no angular stiffness. It says nothing about a transition in real CaB_6 , whose connected octahedra are stiff [25].

The closest community is the study of deformations of homogeneous sphere packings by Fischer, Koch and Sowa, in which sphere packings with free parameters are deformed with their contacts kept, and the $k/m/fn$ types are catalogued [23, 12, 24]. In this language `cab` is the sphere-packing type $5/3/c3$. Sowa described ReO_3 under pressure by the deformation of a sphere packing formed by its oxygen anions [38], Sowa and Ahsbahs studied the cooperative octahedral

tilts of VF_3 -type fluorides under pressure [39], and Sowa and Koch proposed a transition path between the diamond and lonsdaleite types [40]. In the ReO_3 and VF_3 cases the deformation rotates corner-sharing octahedra. The motion here differs in two ways: the octahedra are joined by bridges rather than shared corners and do not rotate, and the symmetry drops from $Pm\bar{3}m$ to $C2/m$ while the lattice deforms, ending at fcc rather than hcp. We have not read every paper in this literature, and a contact-preserving motion of the $5/3/c3$ packing to fcc may already be known there. We make no claim of priority. Periodic flexibility with a variable lattice has a general theory [3, 26], and Borcea and Streinu’s folding sketch [4, Section 7] ends in a folded state of a different realization, not a packing. Ball packings with periodic constraints were studied by Connelly, Shen and Smith [6]; $\pi/\sqrt{18}$ is the maximum density of any sphere packing [19].

6. SUPPORTING RESULTS ON FINITE MOTIONS

In this section balls are joined centre to centre by bars of length $2R$ and may roll on each other.

The plane. The 4.8.8 framework of squares and rods folds into the square tiling; this is the “hinged squares with rods” of Flores [13], who credits Stuart [41], a relative of the rotating-squares mechanism [17]. Alternate squares rotate by $\pm\theta$, the period is $L(\theta) = 2R + 2c\cos\theta$ in both directions, and $\nu = -1$ along the motion, as the criterion of [28] predicts. The closest non-bonded pair has gap $2\sqrt{2}c\cos(\theta+\pi/4)$, so a new contact appears at $\theta = \pi/4$, where the dots form a square lattice of spacing $2R$ and the packing fraction has risen from $\pi(\sqrt{2}-1)^2 = 0.5390$ to $\pi/4$. That no other pair comes closer first was checked numerically, not proved. These are elementary corollaries of a known mechanism.

The cubic-restricted tilt. Rotate the octahedra of $\mathcal{F}_3$ alternately by $\pm\theta$ about $[111]$ and keep the lattice cubic. The bars fix the lattice parameter $a(\theta) = K_1 + \sqrt{4R^2 - 2K_2^2}$, $K_2 = \frac{2}{3}c(1-\cos\theta)$, $K_1 = 2c\cos\theta + K_2$. At $\theta = 60^\circ$, $a = 8c/3$ exactly, each ball has six contacts and the packing fraction is $27\pi\sqrt{2}/256 = 0.4686$. This is a lock of the cubic path, not a jammed state: with a trigonal lattice, states up to 0.648 are connected to $\theta = 0$ on a grid. The six-contact net matches RCSR *sms* in the first ten terms of its coordination sequence; we did not check an isomorphism.

Sampled paths to close packing. A numerical continuation (sequential linear programming with a deformable cell, in the manner of [42], with bar equalities added) found a path of 793 states in a $2 \times 2 \times 2$ supercell from the open state to hcp at $\pi/\sqrt{18}$; two layer slides extend it to pure fcc (1193 states). In the one-cell framework, free descent reached hcp (333 states), and a search steered toward a prescribed fcc end state reached it with density rising at every one of 268 samples. Two checkers written within the project accept all four paths, with consecutive states at most 0.01 apart and interpolated sub-states checked. This is sampled continuity, not a proof; the interpolated paths change bar lengths by up to 2×10^{-5} of $2R$. Greedy density ascent from other starts jammed between 0.58 and 0.71, so the basin that reaches close packing is not generic for this method.

Exact end states. The end states of these paths have exact integer closed forms (in units of K), checked in integer arithmetic: every bar exactly $2R$, no pair closer, 12 contacts per ball, density exactly $\pi/\sqrt{18}$, and hcp or fcc by common-neighbour analysis. In the one-cell fcc end state the octahedron is unrotated in its own frame and the lattice is $L(1)$ of Section 5; the hcp end state has lattice rows $\frac{1}{3}(7, -1, 4)$, $\frac{1}{3}(-4, 7, -1)$, $\frac{1}{3}(-3, 3, 6)$. A certified continuous path to hcp remains open.

7. A RADIUS-RATIO IDENTITY

Let $P \subset \mathbb{R}^n$ be a convex polytope with the origin O in its interior. For a facet F let $\Pi_F = \text{conv}(O \cup F)$, and for a ridge $E = F \cap G$ let W_E be the hyperplane through O and E (the

wall). Suppose each Π_F has an *inscribed ball*, a ball in Π_F tangent to every facet of Π_F , with centre d_F (the *dot*) and radius r_F .

Lemma 5. *If a convex polytope has a ball tangent to all its facet hyperplanes from inside, that ball is its unique largest inscribed ball.*

Proof. Let the facets be $n_k \cdot x \leq h_k$ with unit n_k and the tangent ball $B(x, r)$, so $n_k \cdot x + r = h_k$. If $B(y, r')$ lies inside with $r' \geq r$, then $n_k \cdot (y - x) \leq r - r' \leq 0$ for all k . Since the polytope is bounded there are $\lambda_k > 0$ with $\sum \lambda_k n_k = 0$, which forces $n_k \cdot (y - x) = 0$ for all k and $r' = r$; as the n_k span $\mathbb{R}^n$, $y = x$. $\square$

Theorem 3. *Assume one of the following.*

- (H1) *Every wall W_E is a mirror of P , and Π_F has an inscribed ball for one (hence every) facet.*
- (H2) *P has an insphere centred at O , and the angle φ between the normals of any two adjacent facets is the same for all ridges.*

Then all dots have the same radius r and the same distance D from O ; the balls of two facets sharing a ridge touch, at a point of the common wall; no two balls overlap; and the ball of radius $D - r$ centred at O touches every ball. Consequently the hole/ball ratio is $(D - r)/r = 2D/e - 1$ with $e = 2r$, the classical radius-ratio limit [32] of the polytope Q of dots. Under (H1) P is facet-transitive and Q is vertex-transitive. Under (H2) Q is a scaled polar dual of P , inscribed with all edges equal to $2r$, and $(D - r)/r = 1/\sin(\varphi/2) - 1$; conversely every convex inscribed polytope with equal edges and its circumcentre inside arises in this way.

Proof. (H1). Let ρ_E be the reflection in W_E . It fixes O and E pointwise and permutes the two facets through E . It cannot fix F : the plane of F contains $E \subset W_E$ but not O , so if it were ρ_E -invariant it would be perpendicular to W_E and F would lie on both sides of E in its plane. So $\rho_E(\Pi_F) = \Pi_G$, and by Lemma 5 $\rho_E(B_F) = B_G$. The ball B_F is tangent to W_E at a point fixed by ρ_E , so B_F and B_G touch there, with $r_F = r_G$ and $|Od_F| = |Od_G|$. The ridge graph is connected, so r and D are constant, and the reflections act transitively on facets. Balls lie in pyramids with disjoint interiors, so they do not overlap.

(H2). Let ϱ be the inradius and $\mathbf{n}_F$ the unit outer normal. As O is equidistant from the planes of F and G , W_E is the internal bisector of the dihedral angle at E , with normal proportional to $\mathbf{n}_F - \mathbf{n}_G$, and the angle θ between $\mathbf{n}_F$ and W_E has $\sin \theta = \sin(\varphi/2)$. The point $(\varrho - r)\mathbf{n}_F$ has distance r from the base and $(\varrho - r)\sin(\varphi/2)$ from each wall; these agree for $r = \varrho \sin(\varphi/2)/(1 + \sin(\varphi/2))$, so $D = \varrho - r = r/\sin(\varphi/2)$. The reflection in W_E exchanges d_F and d_G , at distance $2D \sin(\varphi/2) = 2r$. The dots $D\mathbf{n}_F$ are a multiple of the vertices of the polar dual. Conversely, if Q is inscribed with equal edges, its polar has all facets at one distance from O , and the angle between the normals at the ridge dual to an edge qq' is $\angle qOq'$. $\square$

Remark 3 (scope). (1) (H1) holds for the regular polytopes in every dimension, the rhombic dodecahedron, the k -gonal bipyramids of every height, and the Catalan duals of Wythoffian uniform polyhedra. On the rhombic dodecahedron the construction gives the equal-bond UB₁₂ boron net, RCSR ubt. (2) (H2) adds the duals of snub polyhedra and the tetragonal trapezohedron of the single shape dual to the uniform square antiprism. (3) Facet-transitivity and an insphere do not suffice: for tetragonal trapezohedra polar to square antiprisms of height 0.7 and 1.3 times the uniform one, every pyramid has an inscribed ball, but adjacent dots are $[1, 1.017] \cdot 2r$ and $[1, 1.006] \cdot 2r$ apart, so some contacts open. (4) The triangular prism with square sides is not facet-transitive; its pyramids have different inradii and the theorem does not apply. (5) The CN7 and CN9 polyhedra of the radius-ratio tables and the dodecahedral CN8 are not vertex-transitive, so (H1) cannot produce them; under (H2) the triangulated shapes would need to be inscribed equal-edged deltahedra, and the candidates J_{13} , J_{84} , J_{51} are not inscribed. The construction

TABLE 2. Hole/ball ratio of the incentre construction (inscribed balls by linear programming) against the classical radius-ratio limit of Q . All rows satisfy (H1) except the last two, which satisfy (H2).

P	Q (coordination)	hole/ball	classical
tetrahedron	tetrahedron (CN4)	0.2247	$\sqrt{3/2} - 1 = 0.2247$
cube	octahedron (CN6)	0.4142	$\sqrt{2} - 1 = 0.4142$
octahedron	cube (CN8)	0.7321	$\sqrt{3} - 1 = 0.7321$
dodecahedron	icosahedron (CN12)	0.9021	0.9021
rhombic dodecahedron	cuboctahedron (CN12)	1.0000	1
triangular bipyramid, any height	trigonal prism (CN6)	0.5275	0.5275
icosahedron	dodecahedron (CN20)	1.8025	1.8025
tesseract	16-cell (4D)	0.4142	0.4142
pentagonal icositetrahedron	snub cube	1.6874	1.6874
trapezohedron (one shape)	square antiprism (CN8)	0.6453	0.6453

explains one structural limit of the radius-ratio rule; it does not address the softness and size effects behind most of its failures [14]. The script `results/radius-ratio/radius_ratio.py` checks the conclusion on 20 polytopes (Table 2) and the four counterexamples.

8. THE CaB_6 PACKING MAXIMUM

Tiled by the cubic lattice, the dots of the cube are the boron positions of the equal-bond model of CaB_6 [33]: Ca at $1a$ $(0, 0, 0)$, B at $6f$ $(x, \frac{1}{2}, \frac{1}{2})$ and permutations, $x = (\sqrt{2} - 1)/2$. Consider hard spheres of radius r_L on the Ca sites and r_S on the B sites, with x and the lattice parameter a free, and $\gamma = r_S/r_L$.

Theorem 4. *The maximal packing fraction of the CaB_6 structure type at size ratio γ is*

$$\phi_{\max}(\gamma) = \begin{cases} \frac{\pi}{6}(1 + 6\gamma^3), & 0 < \gamma \leq \sqrt{2} - 1, \\ \frac{\pi}{6}(\sqrt{2} - 1)^3(6 + \gamma^{-3}), & \gamma \geq \sqrt{2} - 1. \end{cases}$$

Its global maximum is $\phi^* = \frac{\pi}{6}(30\sqrt{2} - 41) = 0.746865$, attained only at $\gamma = \sqrt{2} - 1$, $x = (\sqrt{2} - 1)/2$, $a = 2r_L$. There the Ca spheres touch each other and each B sphere touches five B spheres, but Ca and B do not touch: $d_{\text{Ca-B}} = 0.73681a > r_L + r_S = 0.70711a$. Moreover $\phi_{\max}(\gamma) > \pi/(3\sqrt{2})$ (fcc) exactly when $(\frac{\sqrt{2}-1}{6})^{1/3} = 0.41023 < \gamma < (4 + 7\sqrt{2})^{-1/3} = 0.41591$.

Proof. Set $a = 1$; then $\phi = \frac{4\pi}{3}(r_L^3 + 6r_S^3)$. Three of the constraints are Ca–Ca, $2r_L \leq 1$; B–B inside an octahedron, $2r_S \leq \sqrt{2}(\frac{1}{2} - x)$; and B–B between octahedra, $2r_S \leq 2x$. The last two give $r_S \leq \min((\frac{1}{2} - x)/\sqrt{2}, x) \leq m^* = (\sqrt{2} - 1)/2$, with equality only at $x^* = (\sqrt{2} - 1)/2$. Hence $\phi \leq \frac{\pi}{6}(1 + 6\gamma^3)$ from $r_L \leq \frac{1}{2}$, and $\phi \leq \frac{4\pi}{3}m^{*3}(6 + \gamma^{-3})$ from $r_S \leq m^*$; the first bound is smaller for $\gamma \leq \sqrt{2} - 1$. Both are attained at $x = x^*$, with $r_L = \frac{1}{2}$, $r_S = \gamma/2$ or $r_S = m^*$, $r_L = m^*/\gamma$, provided no other pair of spheres overlaps. That remaining step is proved by classifying every pair of sites and every lattice translation; the exact minimum distances are $d_{\text{CaCa}} = 1$, $d_{\text{CaB}} = \sqrt{x^2 + \frac{1}{2}}$ and $d_{\text{BB}} = \min(\sqrt{2}(\frac{1}{2} - x), 2x)$, and $r_L + r_S \leq 0.70711 < 0.73681$ throughout [2]. The window follows from $6\gamma^3 > \sqrt{2} - 1$ and $\gamma^{-3} > 4 + 7\sqrt{2}$. $\square$

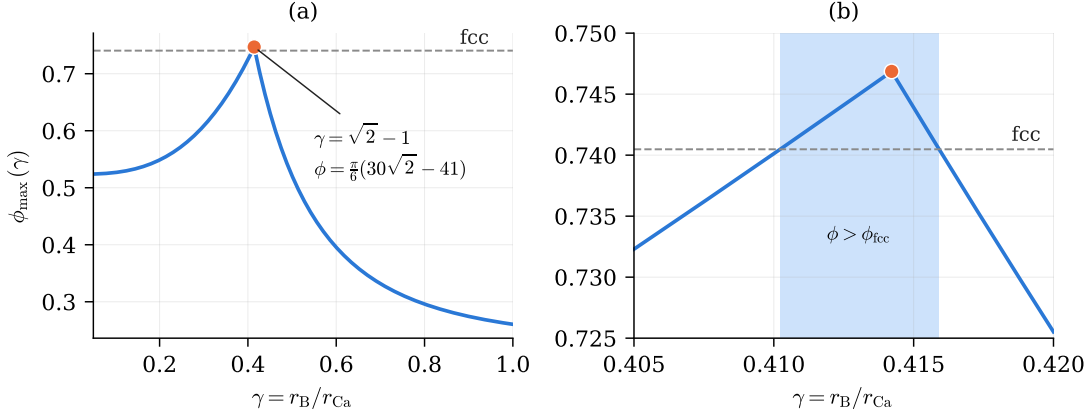


FIGURE 4. (a) Maximal packing fraction of the CaB_6 type versus size ratio (Theorem 4); dashed line: fcc. (b) Detail of the cusp; shaded: the window where it exceeds fcc.

Remark 4. (1) The curve was plotted, for this and 23 other lattices, by Horst and Travesset [21, Fig. 3], and the peak position can be read from their figure. The location $\gamma = \sqrt{2} - 1$ may also be stated by Travesset [43], which we could not read; we did not find the closed form in the sources we read, and we do not claim it is new. (2) The maximum is a cusp (Fig. 4), and the window above fcc is narrow and asymmetric, -0.0040 and $+0.0017$ about $\sqrt{2} - 1$. (3) CaB_6 is not a densest binary packing at this size ratio: the NaCl type reaches $\pi(5 - 3\sqrt{2})/3 = 0.7931$, and CaB_6 is absent from the densest binary packings of [20] and from the Murray–Sanders list of structures beating fcc [29]. CaB_6 -type nanoparticle superlattices are observed [37].

9. OPEN QUESTIONS

Whether the elastic formulas of Theorem 1 are already in the periodic-framework elasticity literature, and whether a contact-preserving motion of the $5/3/c3$ packing to fcc is known in the sphere-packing deformation literature, are the two questions we most want answered by specialists. Mathematically open are a certified continuous path to hcp, a description of the set of close-packed states reachable from the open framework and how they connect, analogous motions in dimensions $n \geq 4$, and the behaviour of these frameworks with angular stiffness. All results here have had internal review only; none has had independent human review.

ACKNOWLEDGMENTS

The drawing began as a doodle the author made on the backs of tests and on napkins, because the pattern was satisfying.

AI assistance: most of the computation, proofs, checking and writing were done by AI models under the author’s direction. Claude models from Anthropic (Claude Opus 5.5 and other Claude models) drafted proofs, code and text, ran the literature searches and the numerical searches for fold paths, and wrote the symmetry-reduced proof of Theorem 2(b) for this version. Some contributions were developed with OpenAI Codex and GPT models: GPT-6 (Codex) derived the explicit curve of Section 5, its first written proof and the first exact certificate, and prepared the all-pairs attainment proof for Theorem 4; GPT-6.1 Sol independently checked the analytic reductions and supplied a second exact implementation; a research assessment prepared with Codex (GPT-6) shaped the priorities of this version. All reviews so far were performed by AI

models under direction; no person other than the author has checked the proofs. Responsibility for the content rests with the author.

CODE AVAILABILITY

Every number in this paper is reproduced by the scripts in the repository <https://github.com/aska-digital/incentre-lattice>, where each result has a folder under `results/` with a written proof (PROOF.md), a deterministic verifier and a certificate; `make verify` replays all of them. The results of v1 are archived in release v1.0.0, doi:10.5281/zenodo.23322080; the additions of this version (`results/fold-continuous-fcc`, `results/cab6-packing/ATTAINMENT.md`) will be archived with the release of this version under the concept DOI 10.5281/zenodo.23322079. Figure 3 is generated from the exact formulas by `papers/source/figures/make_fold_figure.py`.

REFERENCES

1. A. Arifuddin, *An explicit continuous motion from the cab contact framework to fcc: written proof and exact replay*, Folder `results/fold-continuous-fcc` of <https://github.com/aska-digital/incentre-lattice>; to be archived with the v2 release under concept doi:10.5281/zenodo.23322079, 2026.
2. ———, *Maximal hard-sphere packing fraction of the CaB_6 structure type: proof and all-pairs attainment*, Files `results/cab6-packing/PROOF.md` and `ATTAINMENT.md` of <https://github.com/aska-digital/incentre-lattice>; to be archived with the v2 release under concept doi:10.5281/zenodo.23322079, 2026.
3. Ciprian S. Borcea and Ileana Streinu, *Periodic frameworks and flexibility*, Proceedings of the Royal Society A **466** (2010), no. 2121, 2633–2649.
4. ———, *Periodic tilings and auxetic deployments*, Mathematics and Mechanics of Solids **26** (2021), no. 2, 199–216.
5. C. R. Calladine, *Buckminster Fuller’s “tensegrity” structures and Clerk Maxwell’s rules for the construction of stiff frames*, International Journal of Solids and Structures **14** (1978), no. 2, 161–172.
6. Robert Connelly, Jeffrey D. Shen, and Alexander D. Smith, *Ball packings with periodic constraints*, Discrete & Computational Geometry **52** (2014), no. 4, 754–779.
7. J. H. Conway, H. Burgiel, and C. Goodman-Strauss, *The symmetries of things*, A K Peters, Wellesley, MA, 2008.
8. J. H. Conway and N. J. A. Sloane, *Sphere packings, lattices and groups*, 3rd ed., Springer, New York, 1999.
9. H. S. M. Coxeter, *Regular polytopes*, 3rd ed., Dover, New York, 1973.
10. O. Delgado Friedrichs, M. O’Keefe, and O. M. Yaghi, *Three-periodic nets and tilings: semiregular nets*, Acta Crystallographica A **59** (2003), no. 6, 515–525.
11. Rida T. Farouki, *The Bernstein polynomial basis: a centennial retrospective*, Computer Aided Geometric Design **29** (2012), no. 6, 379–419.
12. W. Fischer, *Minimal densities of cubic sphere-packing types*, Acta Crystallographica A **60** (2004), no. 3, 246–249.
13. Alfinio Flores, *Hinged tilings*, North American GeoGebra Journal **6** (2017), no. 1, Section 2.9 and Fig. 9, “Hinged squares with rods”.
14. J. George, D. Waroquiers, D. Di Stefano, G. Petretto, G.-M. Rignanes, and G. Hautier, *The limited predictive power of the Pauling rules*, Angewandte Chemie International Edition **59** (2020), no. 19, 7569–7575.
15. A. M. Glazer, *The classification of tilted octahedra in perovskites*, Acta Crystallographica B **28** (1972), 3384–3392.
16. A. L. Goodwin, *Rigid unit modes and intrinsic flexibility in linearly bridged framework structures*, Physical Review B **74** (2006), 134302.
17. J. N. Grima and K. E. Evans, *Auxetic behavior from rotating squares*, Journal of Materials Science Letters **19** (2000), no. 17, 1563–1565.
18. B. Grünbaum and G. C. Shephard, *Tilings and patterns*, W. H. Freeman, New York, 1987.
19. Thomas C. Hales, *A proof of the Kepler conjecture*, Annals of Mathematics **162** (2005), no. 3, 1065–1185.
20. A. B. Hopkins, F. H. Stillinger, and S. Torquato, *Densest binary sphere packings*, Physical Review E **85** (2012), 021130.
21. N. Horst and A. Travesset, *Prediction of binary nanoparticle superlattices from soft potentials*, Journal of Chemical Physics **144** (2016), 014502, Fig. 3: packing fraction versus size ratio for 24 lattices including CaB_6 .

22. Mats Johansson and Peter Lemmens, *Crystallography and chemistry of perovskites*, Handbook of Magnetism and Advanced Magnetic Materials, Vol. 4: Novel Materials (Helmut Kronmüller and Stuart Parkin, eds.), Wiley, 2007, arXiv:cond-mat/0506606.
23. E. Koch and W. Fischer, *Sphere packings and packings of ellipsoids*, International Tables for Crystallography, Vol. C, Chapter 9.1, International Union of Crystallography, 2006, pp. 746–751.
24. Elke Koch, Werner Fischer, and Heidrun Sowa, *Interpenetration of homogeneous sphere packings and of two-periodic layers of spheres*, Acta Crystallographica A **62** (2006), no. 3, 152–167.
25. Li Li, Keith Refson, and Martin T. Dove, *The contribution of phonons to the thermal expansion of some simple cubic hexaboride structures: SmB_6 , CaB_6 , SrB_6 and BaB_6* , Physical Chemistry Chemical Physics **25** (2023), no. 15, 10749–10758.
26. Justin Malestein and Louis Theran, *Generic combinatorial rigidity of periodic frameworks*, Advances in Mathematics **233** (2013), no. 1, 291–331.
27. J. C. Maxwell, *On the calculation of the equilibrium and stiffness of frames*, Philosophical Magazine, Series 4 **27** (1864), no. 182, 294–299.
28. H. Mitschke, G. E. Schröder-Turk, K. Mecke, P. W. Fowler, and S. D. Guest, *Symmetry detection of auxetic behaviour in 2D frameworks*, EPL **102** (2013), 66005.
29. M. J. Murray and J. V. Sanders, *Close-packed structures of spheres of two different sizes II. The packing densities of likely arrangements*, Philosophical Magazine A **42** (1980), no. 6, 721–740.
30. M. O’Keeffe and B. G. Hyde, *Some structures topologically related to cubic perovskite ($E2_1$), ReO_3 ($D0_9$) and Cu_3Au ($L1_2$)*, Acta Crystallographica B **33** (1977), no. 12, 3802–3813.
31. Michael O’Keeffe, Maxim A. Peskov, Stuart J. Ramsden, and Omar M. Yaghi, *The Reticular Chemistry Structure Resource (RCSR) database of, and symbols for, crystal nets*, Accounts of Chemical Research **41** (2008), no. 12, 1782–1789.
32. L. Pauling, *The principles determining the structure of complex ionic crystals*, Journal of the American Chemical Society **51** (1929), no. 4, 1010–1026.
33. L. Pauling and S. Weinbaum, *The structure of calcium boride, CaB_6* , Zeitschrift für Kristallographie **87** (1934), 181–182.
34. S. C. Power, *Polynomials for crystal frameworks and the rigid unit mode spectrum*, Philosophical Transactions of the Royal Society A **372** (2014), 20120030.
35. Reticular Chemistry Structure Resource, *Nets cab, ubt and sms*, <http://rcsr.net> (raw data file 3dall.txt), Accessed 2026-10-12.
36. Pengfei Shan, Tenglong Lu, Ziyi Liu, Yuanyuan Jiao, Jiajia Feng, Pengtao Yang, Liang Ma, Yoshiya Uwatoko, Xiaoli Dong, Bosen Wang, Bin Chen, Miao Liu, Jianping Sun, and Jinguang Cheng, *Discovery of record-breaking high- T_c superconductivity among 5d transition-metal-oxides up to 17.8 K in ReO_3* , National Science Review **13** (2026), no. 16, nwag425, arXiv:2304.09011.
37. E. V. Shevchenko, D. V. Talapin, N. A. Kotov, S. O’Brien, and C. B. Murray, *Structural diversity in binary nanoparticle superlattices*, Nature **439** (2006), no. 7072, 55–59.
38. H. Sowa, *The oxygen packings of low-quartz and ReO_3 under high pressure*, Zeitschrift für Kristallographie **184** (1988), 257–268.
39. H. Sowa and H. Ahsbahr, *Pressure-induced octahedron strain in VF_3 -type compounds*, Acta Crystallographica B **54** (1998), no. 5, 578–584.
40. H. Sowa and E. Koch, *A proposal for a transition mechanism from the diamond to the lonsdaleite type*, Acta Crystallographica A **57** (2001), no. 4, 406–413.
41. D. Stuart, *Polyhedral and mosaic transformations*, Student Publications of the School of Design, North Carolina State University **12** (1963), no. 1, 2–38, Page range as cited by Flores.
42. S. Torquato and Y. Jiao, *Robust algorithm to generate a diverse class of dense disordered and ordered sphere packings via linear programming*, Physical Review E **82** (2010), 061302.
43. Alex Travesset, *Soft skyrmions, spontaneous valence and selection rules in nanoparticle superlattices*, ACS Nano **11** (2017), no. 6, 5375–5382.