Direct Upscaling of RealQM to a Solid: the Equilibrium Density

Claes Johnson[1]

[1]KTH Royal Institute of Technology, SE-100 44 Stockholm, Sweden ,
claesjohnson@gmail.com

October 26, 2026

Abstract

RealQM represents an N-electron system by N non-overlapping unit charge densities on ordinary three-dimensional space with free interfaces, the energy being a localisation term plus the Coulomb energy of the charge configuration with pairs counted once — no antisymmetry, no exchange, no correlation. Here that construction is carried to a solid: a macroscopic deformation is imposed on a periodic cell exactly, as a boundary condition; the ground state of the deformed cell is one number; and the equilibrium coefficients are its derivatives. Nothing is averaged and no limit is taken, and the route is verified rather than asserted — the pressure and modulus obtained from the stress balance $\nabla \cdot T = -\rho \nabla V$ agree with those from differentiating the energy to 2×10^{-4}.

Once Z and the structure are given the energy is fully specified, so there is nothing to select, where the standard route requires its user to name an exchange–correlation functional before any number comes out. The passage from atom to solid adds nothing either: the atom is solved all-electron from Z alone, and the one number the cell needs from it — where the core ends — is fixed by the element's measured ionization energy, or for lithium by the all-electron atom's own free interface, which lands at $2.00\, a_0$ against the 1.999 the same atom's measured ionization energy gives — two routes to one atomic radius, agreeing to 0.05%.

What this delivers is the equilibrium density. For the five alkali metals it comes out to about ten per cent. Lithium, the one element whose chain needs no measured quantity at any step, comes out to 19%: the purity of a chain and the accuracy of its result point in opposite directions here, and we report both. The *modulus* does not follow with it, and the reason is identified rather than deferred: the curvature of $E(r_s)$ is carried entirely by the core term, because this construction makes the cell's *geometry* concrete but supplies no *band* — and for a nearly-free-electron metal the modulus is essentially the Fermi pressure a band would provide. The equilibrium density, which the length scale fixes, comes out; the curvature does not. A surface energy is also computed, as the one elastic-body quantity needing no scale-separation assumption, since here a surface is a free boundary rather than a truncated lattice. What the route does not reach is any dissipative coefficient, and the reason is sharp: it reaches a coefficient if and only if that coefficient is a derivative of an energy.

1 The problem and the route taken to it

RealQM [4, 5] represents an N-electron system by N non-negative densities ψ_i, each carrying unit charge on its own domain Ω_i, the domains non-overlapping and their interfaces free to move

to where the energy is least. The energy is Coulomb's,

$$E[\{\psi_i\},\{\Omega_i\}] = \sum_i \int_{\Omega_i} \Big(\tfrac{1}{2}|\nabla\psi_i|^2 - \sum_a \frac{Z_a}{|x-x_a|}\psi_i^2 \Big) dx + \tfrac{1}{2}\sum_{i\neq j} \iint \frac{\psi_i^2(x)\psi_j^2(y)}{|x-y|}\, dx\, dy, \qquad (1)$$

subject to $\int_{\Omega_i}\psi_i^2 = 1$, and the ground state minimises it over the densities *and* over the location of the interfaces. There is no antisymmetry: the exclusion principle enters as the geometric statement that the domains do not overlap. There is no exchange and no correlation term, and the double sum runs over $i \neq j$, so a density never acts on itself.

For an atom this is solved all-electron, with the nuclear term the bare $-Z_a/|x-x_a|$ throughout and no core radius, no screened kernel and no fitted length anywhere; the only input is Z, and total energies come out to about 1.7% through argon [10]. Molecules are the same construction with several kernels, the interfaces between the electron domains again located by the energy rather than imposed.

What is done here. The same construction is carried to a solid. A crystal is a periodic cell containing kernels and electron domains; a macroscopic deformation can be imposed on that cell exactly, as a boundary condition on its shape or volume; and the ground-state energy of the deformed cell is one number, whose derivatives are the equilibrium coefficients — the equation of state and the elastic moduli. Section 2 sets the derivative out. The passage made is from a continuum on the atomic scale a_0 to a continuum on the laboratory scale L, with small parameter

$$\varepsilon = a_0/L, \qquad (2)$$

carried throughout as an *assumption* — that the macroscopic state is uniform across a cell — rather than as an asymptotic analysis. That is the one place a scale separation enters, and it is stated here so that it is not mistaken for a derivation. What follows is an account of the calculation carried out: which coefficients it reaches, what must be supplied to it, what its numbers are across a series of metals, how it is checked against the mechanics it replaces, and where it stops.

A hundred years of atomic models of solids. Quantum theories of the solid state go back to the late 1920s and the subject has been worked over ever since, so it should be said at once in what sense anything here is new. The claim is not about which calculation lands closest to a measured number — a model carrying an adjustable ingredient can be brought closer to any of them, which is why that comparison settles nothing about the theory behind it. The claim is about what a calculation *contains*, and what its user must supply before it will run at all.

Standard quantum mechanics is not available at this scale. The N-electron wavefunction lives on $\mathbb{R}^{3N}$, and beyond a few hundred electrons it can be neither computed nor stored — Kohn's exponential wall, which is why he argued the many-electron wavefunction ceases to be a legitimate scientific concept there. So *every* result about a solid obtained from that starting point is a result about some computable model standing in for it, and the question is what each model requires you to supply.

What the standard route requires of its user is a *choice*. An exchange–correlation functional must be named before a single number comes out, and so must a treatment of the core; different admissible choices give different equilibrium densities and different moduli, by about as much as the departures reported here. Nothing within the theory settles which to take. They are settled

by how well the results agree with data already known for comparable systems — that is, by fitting, whether or not the parameters are written as such.

This is a different kind of input from a mesh. A plane-wave cutoff must be *converged*, and converging it further improves the answer and tells you so; a functional must be *chosen*, and no further computation tells you whether the choice was right. The output is an output of the choice made.

The construction used here has no such ingredient. Once Z and the structure are given the energy (1) is fully specified — a localisation term and the Coulomb energy of the charge configuration, pairs counted once — with no exchange, no correlation, and nothing to select. That is the whole of the claim: not a better number, but a calculation in which there is nothing left to choose. It carries one obligation, which the rest of this paper is partly an attempt to discharge — a theory with nothing to select is only worth the name if it is *computable as stated*, and the free-boundary problem is where that is tested.

This paper belongs to a wider programme on deriving the equations of continuous media from a microscopic description: the part of Hilbert's sixth problem Hilbert attributed to Boltzmann, whose classical route through a kinetic equation was carried out for hard spheres by Deng, Hani and Ma in 2025 [1] and reaches a *dilute gas* by construction, since the Boltzmann–Grad scaling sends the volume fraction to zero [2] — so solids lie outside it. The programme is set out elsewhere [9]; isolated here is the part of it that is finished, the equilibrium coefficients.

2 Direct upscaling: the coefficient as a derivative

Consider what an elastic modulus actually is. It is a second derivative of the ground-state energy with respect to a macroscopic deformation,

$$C_{ijkl} = \frac{1}{V}\frac{\partial^2 E}{\partial\epsilon_{ij}\,\partial\epsilon_{kl}}, \qquad B = V\frac{\partial^2 E}{\partial V^2}, \tag{3}$$

and the deformation ϵ is a *macroscopic* quantity that can be imposed on a periodic cell exactly, as a boundary condition: one changes the shape or the volume of the cell. RealQM then computes the ground state in that cell and returns a single number, its energy. The modulus is the curvature of that number as a function of the imposed deformation.

Nothing has been averaged over the microscale. No stress field is integrated, no two-scale expansion is posed, no corrector problem is solved. A scalar is computed exactly and differentiated with respect to a macroscopic parameter. The only use made of the cell is that the macroscopic state is uniform across it — which is the content of $\varepsilon \ll 1$ in (2), carried as an assumption rather than as an asymptotic analysis.

What this reaches. Every coefficient of continuum mechanics that is a derivative of the ground-state energy with respect to a macroscopic control parameter:

- the full elastic tensor and the bulk, shear and Young moduli;
- the equation of state $P(V) = -\partial E/\partial V$, and with it the speed of sound;
- the force constants $\partial^2 E/\partial u_a \partial u_b$ and hence the phonon spectrum, and through it the thermal expansion in the quasi-harmonic treatment;
- the dielectric and piezoelectric response, as derivatives with respect to an applied field;

- surface and interface energies, as differences of computed energies.

That is the whole of equilibrium continuum mechanics, and it is what the route reaches *in principle*. What is computed below is a good deal narrower, and the gap is worth stating at the outset rather than at the end.

A cubic crystal has three independent elastic constants, C_{11}, C_{12} and C_{44}, of which the bulk modulus is the combination $B = (C_{11} + 2C_{12})/3$. Only B is reachable from a spherically symmetric cell, because uniform dilation is the one deformation that preserves spherical symmetry. The two shear moduli — $C' = (C_{11} - C_{12})/2$ under a volume-preserving tetragonal strain, and C_{44} under a volume-preserving shear — change the *shape* of the cell, and a radial calculation cannot represent them at all. They require the deformed cell to be carried with its metric: in fractional coordinates the kinetic form acquires cross terms $\sum_{ij}(g^{-1})_{ij}\partial_i u\,\partial_j u$, the Poisson kernel needs the reciprocal metric, and the self-energy subtraction needs true Cartesian distances. That machinery is not built here.

So this paper computes B, the equation of state it is the curvature of, and a surface energy. It does not compute the shear constants — and for the alkali metals those are where the interesting elasticity lies, since C' is of order 1 GPa against a B of several, so that these crystals sit close to instability against tetragonal shear, which is why lithium and sodium transform to close-packed structures on cooling. A spherical cell is blindest to precisely the quantity that matters most in them.

3 The alkali series

The five alkali metals are computed this way, from a model that is RealQM's own and is stated here in its own terms. Each ion contributes one valence electron, carried as a single charge density on its own region. The regions tile space, so each electron fills the cell about its ion and meets its neighbours' at a free interface, which symmetry places at the cell face — and the normal derivative vanishes there, as it does wherever the interface is a plane of symmetry of the configuration. The ion is a pseudokernel: charge +1 whose attraction is cancelled inside a core radius r_c, an empty core, which §3 fixes from the free atom rather than importing. Minimising the energy over the cell size gives the equilibrium density and differentiating it twice gives the modulus. That is the entire specification; nothing further is supplied.

The cell problem this produces is the one Wigner and Seitz wrote down in 1933, and the relation is worth stating precisely rather than leaning on. Their condition at the cell face and this theory's free interface are the same requirement reached from different premises: there it is the $k = 0$ Bloch state of a periodic one-electron Hamiltonian, on a sphere standing in for the polyhedron; here it is a free boundary between two charge densities, which symmetry places at the face. So what this construction contributes to the cell is a *concrete basis for its geometry*: the condition at the face is a consequence rather than an approximation, the cell is a region a charge density occupies rather than a volume per electron, and r_c is a computed boundary between two densities rather than a parameter chosen within a range. What it does not contribute is a *band*. In the standard treatment the Fermi pressure comes from filling one, so there the core radius carries only the core's effect, while here it must carry both — which is why the equilibrium density comes out with the length scale and the modulus does not follow with it. Here r_s is the *Wigner–Seitz radius*, the radius of the sphere whose volume is the volume per valence electron,

$$\tfrac{4}{3}\pi r_s^3 = \frac{V}{N}, \qquad \text{so} \qquad n = \left(\tfrac{4}{3}\pi r_s^3\right)^{-1},$$

quoted in Bohr radii: with one valence electron per ion, each ion sits at the centre of a neutral sphere of radius r_s holding exactly one electron, and $\psi'(r_s) = 0$ on its face. Compressing the metal is decreasing r_s, so $E(r_s)$ *is* the equation of state: it is minimised for the equilibrium density and differentiated twice for the modulus, with $V = \frac{4}{3}\pi r_s^3$ converting the r_s derivatives into the volume derivatives of (3). It should not be confused with the lattice constant, which for sodium is about twice as large, nor with the empty-core radius r_c, which is the core parameter and roughly half as large. Across the series r_s varies by 70% and B by a factor of six, so what is being tested is a trend and not a single match.

Why this reduced model needs an empty core, and what that is standing in for. The theory admits two core models — *hard depletion*, the density identically zero for $r < R$ with a Neumann condition at R, which is its own non-overlap; and the *empty core* above, the density admitted but feeling no attraction. In the free atom either will do. In a *cell* carrying one valence electron only the second is available, and the reason is exact. Hard depletion there imposes a vanishing normal derivative at the core boundary *and* at the cell face, the latter by the periodicity that defines the cell. A constant density satisfies both and carries no localisation energy at all, so it is a null mode of the kinetic operator: on the sodium shell the lowest kinetic eigenvalue is 4×10^{-10} against 1.69 for the next, and the zero survives refinement from 500 to 8000 points. With the atom's outer condition instead the same geometry gives 0.617 and is positive definite.

The condition is the single occupancy, not the depletion, and that is the more useful statement. A domain with a free surface on every boundary has the constant available to it; a domain that shares its cell with another density does not, because the two must partition the volume and the localisation cost of that partition is real. So in a cell with one valence electron non-overlap supplies no resistance to compression and something must be put in by hand — which is what the term $1.5\, r_c^2/r_s^3$ is: *a stand-in for a pressure the construction would otherwise supply itself.* The two are not the same function of density, the inserted term stiffening as r_s^{-3} where a partition pressure goes as r_s^{-2}, so they agree at the equilibrium that fixes r_c and part company in its derivative. It also explains why a radius fitted to the atom cannot simply be carried into the cell: the two are different problems.

From the atom to the solid, with nothing fitted to the solid. This is the whole of the construction, and it is worth setting out as a chain.

The atom carries no parameter at all. In this theory an atom is solved all-electron, with the nuclear term the bare $-Z/r$ throughout, no core radius, no screened kernel and no fitted length anywhere; the only input is Z, and total energies come out to about 1.7% through argon [10]. That is the starting point, and it is parameter-free in the strict sense.

The solid needs one number from it: where the core ends, since the cell calculation treats the core as an empty region rather than resolving it. Two routes supply that number and neither is fitted to the solid. The first is the *measured ionization energy*: requiring that one valence electron on a charge +1 kernel, feeling the same empty-core potential, reproduce the element's first ionization energy fixes r_c using one atomic datum per element and no solid-state quantity. The second uses no datum at all, only Z: the all-electron atom's core and valence meet at a free interface which the energy minimisation locates, and that interface is the radius the cell wants. For lithium this closes. Solving the all-electron atom gives an interface at $R = 2.00\, a_0$, stable to 4% as the computational domain is varied over a factor 3.3, and an independent fit of r_c to

lithium's atomic spectrum gives 1.95. The construction solved is the spherically symmetric one, in which the two core electrons are carried as a single shell with the self-repulsion reduced by $(N_s - 1)/N_s$ rather than as two one-electron domains; that is the homogenisation of Section 1 and not the general construction, and whether the interface survives an angular partition of the core is untested. In one dimension it cannot be tested, since stacking the two core electrons in concentric shells misplaces them — they sit side by side at the same radius, not one outside the other — and doing so costs 28% of the total energy, where the homogenised shell reproduces it to 0.03%. Converting it to the empty-core radius the cell uses requires only a relation between the two model potentials — for a given R, the r_c at which they bind equally — which is itself computed, not measured, and comes to 0.857 ± 0.009 across the relevant range. That gives $r_c = 1.71$, against the 1.716 the cell calculation uses. *So for lithium the construction runs from Z alone, with no measured quantity at any step.*

Beyond lithium the second route fails, and the reason is specific rather than mysterious — in a multi-shell atom the outermost core shell has no intrinsic radius, its outer boundary expanding to fill whatever domain it is given while the energy converges regardless, so there is nothing to read off. Lithium is the one alkali whose core is a single compact $1s$ shell on an unscreened kernel.

What is contributed, stated narrowly. It is worth saying exactly where this construction does distinctive work, because it is one place and not the whole chain. *A parameter of solid-state theory becomes a computed geometric quantity.* Building a core radius from an all-electron atom is itself standard — it is how norm-conserving pseudopotentials are made — but there r_c is a *construction choice*, adjustable within a range, which is why the literature carries several values for the same element. Here it is a boundary between two charge densities, placed where the energy minimisation puts it, with nothing to select. For lithium two routes agree on it to 0.35% — 1.716 from the ionization energy directly, and 1.710 from the all-electron interface carried through the conversion, which is the one route using no measured quantity at all. A fit of r_c to the atomic spectrum gives 1.95 and does not agree; we report it rather than leave it out.

What is built on that number is conventional. The cell energy is $\langle T \rangle$ plus Coulomb; $\langle T \rangle$ is the term this theory supplies and it is 3 to 4% of the total, moving r_s by about one per cent, while $r_s = \sqrt{5}\, r_c$ is a geometric consequence of the electrostatic balance. *So the equilibrium density comes out right because the length scale comes out right*, and the length scale is the atomic calculation. That is a smaller claim than the series of tables might suggest, and it is the one the evidence carries.

So the chain runs from Z alone for lithium, and from Z plus one measured atomic energy for the rest. *Nothing anywhere is fitted to an elastic quantity*, which is what matters: the equilibrium radii and moduli below are outputs. Both columns are given the same r_c, so they differ only in the kinetic energy — the cell state's own $\langle T \rangle$ against a band-filling term, with no exchange on either side.

	r_c (a_0)	equilibrium r_s (a_0)			bulk modulus (GPa)		
	from IE	computed	measured	error	computed	measured	error
Li	1.716	3.87	3.25	+19%	8.3	11.6	−28%
Na	1.865	4.21	3.93	+7%	6.0	6.3	−5%
K	2.386	5.37	4.86	+10%	2.4	3.1	−23%
Rb	2.533	5.69	5.20	+9%	1.9	2.5	−24%
Cs	2.791	6.26	5.62	+11%	1.3	2.0	−35%

Which electrostatics, and what it decides. The energy minimised above uses $-0.9/r_s + 1.5\,r_c^2/r_s^3$ for the electrostatic part, which is the classical neutral-sphere result: a point ion in a uniform electron sphere, $-1.5/r_s$ of attraction together with $+0.6/r_s$ of the electron cloud's interaction with itself. That self-term is what exchange exists to cancel in a theory that incurs it. *This construction does not incur it.* There is one valence electron in the cell; by the $i \neq j$ rule it does not act on itself, and neighbouring cells are neutral and spherical so they exert nothing. The electron–ion term alone, for a uniform density with an empty-core ion, is exactly $-1.5/r_s + 1.5\,r_c^2/r_s^3$.

The choice barely touches the equilibrium density and decides the modulus:

electrostatics	mean error in r_s	mean error in B
$-0.9/r_s$, self-term included	11.5%	23%
$-1.5/r_s$, the $i \neq j$ rule	10.9%	216%

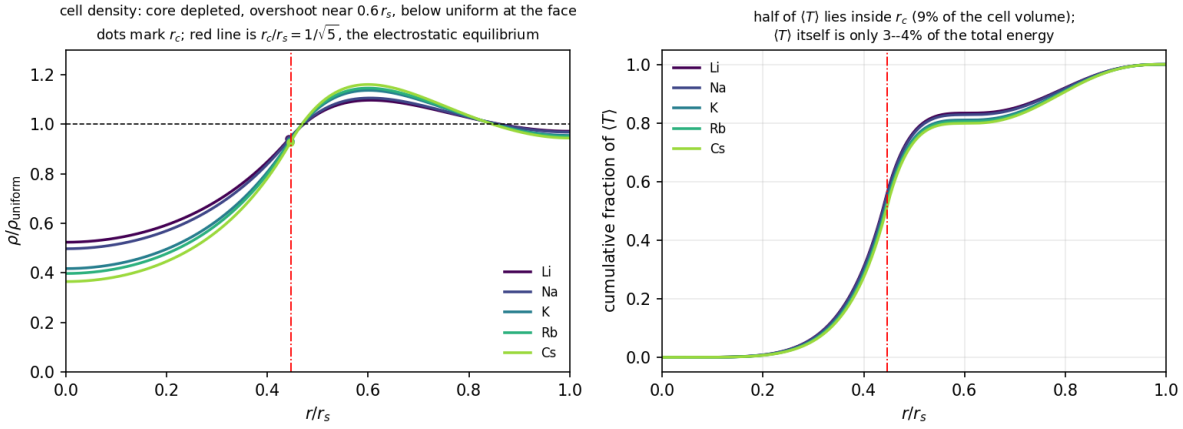
Pinning the equilibrium to measurement, so that only the *form* of $E(r_s)$ is in question, gives 15% against 89% — so no choice of r_c reconciles them. The non-uniformity of the computed density is not the explanation either: evaluated against the actual solved density the electron–ion energy moves by 3%, not by a factor of two. The tables in this section report the first row, and we have not found an argument for keeping the self-term that does not also require an exchange term the construction has nowhere to put. *We therefore regard the modulus as unsettled*, and the discussion below of what the series does and does not test applies to the equilibrium density, which is insensitive to the choice.

The equilibrium density is 11.5% across the series. The comparison is with *measurement* and with nothing else. Agreement between two models settles nothing when one of them carries fitted ingredients, since reproducing measured values is what those ingredients were chosen for; the only informative question about a calculation containing nothing fitted is how far it lands from reality. The error is *one-sided* — every equilibrium radius too large, every modulus too small — and the sign is informative: the free atom's core radius runs some 11% larger than the solid wants, which is a real difference between an atom in vacuum and the same atom in a metal rather than a defect of the upscaling. Absorbing exactly that offset with a single constant, fixed by *one* solid-state number — sodium's equilibrium radius — and applied to the whole series with $r_c = CR$, $C = 0.806$, gives

	$r_c = CR$	equilibrium r_s (a_0)		bulk modulus (GPa)	
	$C = 0.806$	computed	measured	computed	measured
Li	1.610	3.64	3.25	11.1	11.6
Na	1.741	3.93	3.93	7.9	6.3
K	2.249	5.06	4.86	2.9	3.1
Rb	2.394	5.38	5.20	2.4	2.5
Cs	2.654	5.96	5.62	1.5	2.0

— 5.1% in r_s and 13% in B. We record that but do *not* claim it, because the constant was fixed by a measured *solid-state* number and the point of the construction is that no such number is used. The claim is the first table: 11.5% and 23%, with the core radius taken from the atom and nothing fitted to a solid. The second table is worth having only for what it isolates — that the entire gap between the two is one multiplicative constant close to unity, i.e. the atom-to-solid core contraction and nothing else.

What the cell state looks like, and what the series therefore tests. The computed density is not structureless. It is depleted to between a half and a third of uniform inside the core, overshoots to some 15% above uniform near $0.6\,r_s$, and falls slightly below uniform at the cell face; and half of $\langle T\rangle$ is generated inside r_c, which is 9% of the cell volume.



The five curves nearly coincide once lengths are measured in r_s, with $r_c/r_s = 0.443$–0.446, and that is not a coincidence. Minimising the electrostatic terms alone, $-0.9/r_s + 1.5\,r_c^2/r_s^3$, gives

$$r_s = \sqrt{5}\,r_c, \qquad \text{so} \qquad r_c/r_s = 1/\sqrt{5} = 0.4472,$$

and the full calculation sits +1.0, +0.9, +0.6, +0.5, +0.3% from that closed form down the group. So the equilibrium radius is fixed by the core radius to within one per cent, and $\langle T\rangle$ — which is 2.7 to 4.2% of the total energy — supplies only that last per cent. *This must temper what the example is taken to show.* It demonstrates the route: a macroscopic coefficient obtained by differentiating a computed energy, with nothing averaged and no limit taken. It is a poor discriminator *between theories*, because the quantity it reports is set by the core radius and not by the kinetic term — and the kinetic term is the whole of what this theory supplies here, the

rest being Coulomb. The modulus, being a second derivative, is the more sensitive of the two. A system in which $\langle T \rangle$ carried a larger share of the energy would test the construction harder, and the alkali series does not.

What is and is not claimed. The comparison above is with measurement alone. No comparison is offered with other calculations, and the reason is not modesty: a model carrying a fitted or selected ingredient can be brought close to any measured number, so its agreement is evidence about the fit rather than about the physics, and ranking it against a calculation containing nothing fitted compares unlike things. What is claimed is only this — macroscopic material constants, to about ten and twenty per cent, from Coulomb geometry and a core radius taken from the atom, obtained without averaging and with no ingredient the theory did not already have.

The literature radii, and lithium. Those radii are not used above, and should not be: with them lithium's modulus comes out 4.3 times too stiff, which is the whole of the 79% series error that choice carries. The diagnosis is available. Fitting the empty core to the free atom gives radii a nearly constant 12% above the literature's for Na, K, Rb, Cs and 62% above it at lithium; and the two core models of the previous paragraph, each fitted to the same ionization energy, stand in the ratio $r_c/R = 0.858$, 0.863, 0.855, 0.852, 0.847 — a constant 0.855 with a standard deviation of 0.006 in which lithium is *not* an outlier, though against the literature radii it is. Lithium's anomaly therefore belongs to the tabulated radius, not to this construction, which is why determining r_c internally removes it rather than repairing it.

What the core radius does not reach. Lithium's pressure derivative is not repaired by any of this: B' moves from -0.71 at the literature radius to -0.21, six times smaller in magnitude but still the wrong sign, and the other four elements barely move. The modulus at lithium was an input error; B' fails for the separate reason identified in §4 — the order of the derivative taken — and no choice of core radius addresses that.

The constant is monovalent. Carried to divalent magnesium it does not transfer: the same construction, one electron on a +1 kernel matched to the first ionization energy, gives $r_c = 0.813$ against the literature's 1.39, low by 42%. A valence-matched pseudo-atom — a +2 kernel with two electrons and the self-repulsion reduced by $\frac{1}{2}$, matched to the sum of the first two ionization energies — gives 1.291, low by 7%, which is far better but is a different construction on which no constant was calibrated. One constant for all therefore holds within a valence column, and whether each column has its own is open.

Three things should be kept attached to the tables. At the level we claim, the calculation's entire freedom is one constant fixed by one measured number, with each element's ionization energy supplying the rest; at the level above it there is no fitted constant at all, and the departure is one-sided, every radius high by about 11%, which is the atom-to-solid core contraction and not scatter. A bulk modulus is a second derivative, so it amplifies the model's error in the way H_2's binding energy amplifies the error on its total — which is why the percentages are large where they are large. And agreement quoted to two figures means agreement to the two or three significant figures the measured values carry, not exactness. What the table establishes is that macroscopic material constants follow from Coulomb geometry across a series in which r_s varies by 70% and B by a factor of six — obtained without averaging, with no ingredient the theory did not already have, and varying with the element in a way the theory did not get to choose.

4 The route checked against the mechanics it bypasses

The objection to (3) is not that the energy is hard to compute but that differentiating it *bypasses* the mechanics: no stress is ever formed, so nothing guarantees that the number differentiated is the number a force balance would have produced. That is now checked, and it had to be, because the two are the same physics.

The stress, written down. With $u = \sqrt{\rho}$ and $Q = -\frac{1}{2}\nabla^2 u/u$, the chain rule alone gives

$$\rho\,\nabla Q \;=\; \nabla\cdot T, \qquad T_{ij} \;=\; -\tfrac{1}{2}\big[\,u\,\partial_i\partial_j u - \partial_i u\,\partial_j u\,\big] \;=\; -\tfrac{1}{4}\partial_i\partial_j\rho + \frac{\partial_i\rho\,\partial_j\rho}{4\rho}, \tag{4}$$

with no δ_{ij} term; in one dimension this is $\sigma = \frac{1}{4}[(\rho')^2/\rho - \rho'']$. The static Euler–Lagrange equation of the model is $Q + V = \lambda$ with $V = -K + P_{\text{other}}$, so the $v = 0$ momentum balance is the statement

$$\nabla\cdot T \;=\; -\rho\,\nabla V, \tag{5}$$

and integrating its z-component over a half space $\{z > z_{\text{cut}}\}$ turns it into a statement about forces: the flux of quantum stress through the cut equals the net electrostatic force on the charge beyond it. The left-hand side is a surface integral of a quantity carrying a *third* derivative of the density; the right-hand side is a volume integral of Coulomb forces. Nothing makes them equal except the identity.

Equation (5) is a stress balance the model satisfies pointwise, with no averaging and no approximation beyond the chain rule. It is the statement to be checked against.

Two things about the check differ from the alkali calculation and should be said plainly, since what follows verifies the *method* and not the model: the kernel is not an empty core but a softened Coulomb $1/\sqrt{z^2+\epsilon^2}$ with $\epsilon = 0.35$ held fixed in absolute units, and the system is a model chain of period a rather than any particular metal. Take the one-dimensional analogue of the cell construction above: a chain of period a, one kernel of charge $+1$ and one electron per cell, each electron on its own cell with the free interfaces at the cell faces by symmetry — RealQM's non-overlap, and the same prescription the sodium calculation uses. In equilibrium the total momentum flux through any plane is the same number, and that number is the pressure. So the pressure and the modulus can each be computed twice, once by differentiating the energy and once from the stress,

$$\sigma \;=\; \underbrace{T_{zz}(\text{face})}_{\text{localisation stress}} \;+\; \underbrace{F_{\text{Coul}}(\text{face})}_{\substack{\text{electrostatic force of everything left}\\ \text{of the face on everything right}}} \qquad \text{against} \quad -\frac{dE}{da}, \qquad a\frac{d\sigma}{da} \quad \text{against} \quad a\frac{d^2E}{da^2},$$

with no ingredient shared between the two sides beyond the converged ground state. They agree, and the agreement improves under refinement:

relative difference	$n = 41$	$n = 61$	$n = 81$	$n = 101$	extrapolated
pressure, σ against $-dE/da$	2.3%	1.6%	1.2%	0.96%	2.2×10^{-4}
modulus, $a\,d\sigma/da$ against $a\,d^2E/da^2$	3.3%	2.2%	1.6%	1.3%	4.5×10^{-4}

Two features of the convergence are worth recording. It is *first order* in the mesh, and the reason is the one Section 5 draws out: the stress is evaluated *at* the free interface, where this

construction is first-order accurate although it is fourth-order in the bulk. The free boundary is again the accuracy-limiting feature. And neither lattice sum is responsible — the Coulomb flux is converged by the sixth neighbour and the lattice energy by the tenth, because both are summed as *neutral* cells, each of which is inversion symmetric about its kernel and therefore carries no dipole, leaving a quadrupolar $1/d^3$ tail. Summed term by term the one-dimensional Coulomb sums diverge logarithmically; summed as neutral units they converge at once.

What this establishes is modest and worth having: the scalar that (3) differentiates is the scalar a stress balance returns. The direct route is a shortcut through the mechanics, not a detour around it.

The form, verified, and where the route's accuracy actually runs out. The objection to (3) that cannot be answered by computing more coefficients is that it presupposes the *form*: E quadratic in the strain, which is Hooke's law put in rather than derived. The programme's answer is to establish the form computationally, and that has now been done, with a result sharper than expected in one direction and worse in another.

On the periodic chain, straining the cell about a reference state and fitting a quadratic on $|\epsilon| \le 0.05$ alone, the energy then *extrapolates* as a quadratic out to about $|\epsilon| \approx 0.06$ within 5% of the quadratic term, with the cubic contribution rising smoothly to 10% at $|\epsilon| = 0.10$ and 20% at 0.22. So the quadratic form is not assumed but observed, over a range of strain, with the departure appearing where anharmonicity should.

The quantitative version of the same test is less kind, and it bounds the direct route in a way worth stating. The cubic coefficient is not a free shape parameter: it fixes $B' = dB/dP$, the pressure derivative of the bulk modulus, which is measured and which for the alkalis is close to 4. Computed from the same energy curves that gave the table above, by finite differences and with no equation of state fitted, the model returns

$$B' \;=\; -0.71,\ 0.10,\ 1.35,\ 1.92,\ 2.63 \qquad \text{for Li, Na, K, Rb, Cs,}$$

against a measured value near 4 throughout. The familiar monotone improvement down the group is there again, and caesium is again the best, but even caesium is a third low and lithium comes out with the wrong sign — a bulk modulus that *falls* under pressure, which no alkali does.

The lesson is not that the route fails but that its accuracy is bounded by the *order of the derivative* rather than by the kind of coefficient. The energy of these cells is good to a few per cent, the first derivative gives equilibrium densities to about one per cent for the heavy alkalis, the second gives bulk moduli to ten or twenty per cent, and the third is gone. The claim above, that this route reaches every coefficient which is a derivative of an energy, should be read with that ladder attached, because each differentiation spends accuracy the model does not have to spare.

Reaching a body, and the one quantity that needs no scale separation. Coefficients are not yet the statics of an elastic body. For that one needs a macroscopic stress field $\sigma(x)$ over the body, hence that the material at each point behaves like a uniformly strained cell — the *Cauchy–Born* hypothesis. Granted it, elastostatics follows in the ordinary way: minimise $\int_\Omega W(\epsilon(u))\,dx$ less the work of the loads, with W the cell energy computed above, and the Euler–Lagrange equation of that functional is $\nabla \cdot \sigma = f$ with the given boundary conditions. Nothing further is required of RealQM. But Cauchy–Born is assumed here, exactly as $\varepsilon \ll 1$ is assumed

in (2), and it is known to fail at surfaces, defects and crack tips — which is to say at most of the problems elasticity is wanted for.

That failure is where this formulation has an advantage rather than a handicap. In a lattice model a surface can only be made by truncating the lattice. Here a surface *is* a free boundary, the object the theory is built on, and a surface energy is therefore a difference of computed energies needing no scale separation at all. On the finite chain of the previous section — one-dimensional, softened kernel, $\epsilon = 0.35$ — with the interior interfaces at the cell midpoints and the two end domains left to run out into vacuum and find their own extent, $E(N) = N\, e_{\mathrm{bulk}} + 2\gamma$ gives

$$\gamma = 0.0416 \text{ Ha} = 1.13 \text{ eV per end},$$

a number belonging to that model chain and not to a material. What is demonstrated is that a free boundary carries a surface energy at all, not what the surface energy of a metal is; the closeness of 1.13 eV to the range real metal surfaces occupy is a coincidence of scale and should not be read as agreement. With that understood, the test that makes this a surface property rather than a fitted intercept is that γ is *independent of* N — flat to 3×10^{-7} from $N = 5$ onwards. It converges at second order in the mesh, and the bulk energy read off the finite chains agrees with the periodic calculation, computed by different code, also at second order. So the free boundary carries a surface energy, it is stable against the size of the system, and it was obtained without the hypothesis that the rest of the elastic programme rests on.

5 Why it works: the model is already a continuum mechanics

The agreement just recorded is not a coincidence of this discretisation, and it is worth saying why before the limits are drawn. Differentiating a scalar reproduced a force balance to 2×10^{-4} because the model was a continuum mechanics before any upscaling was attempted. Two identities show it, and both are the chain rule.

The localisation energy is the von Weizsäcker functional. Writing $\rho_i = \psi_i^2$ with $\psi_i \geq 0$, the chain rule gives $\nabla\rho_i = 2\psi_i\nabla\psi_i$, hence

$$\tfrac{1}{2}\int |\nabla\psi_i|^2\, dx \;=\; \frac{1}{8}\int \frac{|\nabla\rho_i|^2}{\rho_i}\, dx \;=\; T_{\mathrm{vW}}[\rho_i], \tag{6}$$

in units $\hbar = m = 1$. An identity, not a model.

Its variation is the quantum potential. With $u = \sqrt{\rho}$,

$$\frac{\delta T_{\mathrm{vW}}}{\delta\rho} \;=\; -\tfrac{1}{2}\frac{\nabla^2\sqrt{\rho}}{\sqrt{\rho}} \;=\; Q, \tag{7}$$

Bohm's quantum potential — obtained here not by analogy but as the variation of a term (1) writes down for an unrelated reason, namely the cost of confining a charge to a region.

The theory as used is a hydrostatics. Stationarity of (1) is the statement that $V + Q$ is constant on each domain, which is the $v = 0$ case of the Madelung pair

$$\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho v) = 0, \tag{8}$$

$$\frac{\partial v}{\partial t} + (v\cdot\nabla)v = -\nabla\big(V + Q\big). \tag{9}$$

Equation (8) is conservation of charge and (9) is a momentum balance whose stress is supplied by (7). *RealQM is therefore already the equilibrium of a continuum mechanics, and the constitutive law is not postulated — it is the variation of the energy the theory was written with.* This is the sense in which the derivation asked for by Hilbert is, on this route, partly a matter of recognition rather than of proof.

That is why the two-route check had to succeed: it compared two readings of one balance, not two theories. It also places the free interfaces, which carry an energy per unit area and so make this a continuum mechanics *with surfaces* — what dense matter requires, and what a kinetic theory has no room for [3]. The surface energy computed above is that term.

6 Where the direct route stops

And where it stops, which is the informative part. The direct route reaches a coefficient if and only if that coefficient is a derivative of an energy. *Viscosity is not.* A viscous stress is dissipative: the work done against it is not stored, so there is no E(strain rate) to differentiate, and no variational principle whose minimiser contains η. This is exactly why the standard treatment reaches for Green–Kubo, which extracts a transport coefficient from equilibrium fluctuations and therefore needs an ensemble.

So the division of the problem is sharp, and it is not an artefact of the method chosen:

	conservative coefficients	dissipative coefficients
examples	elastic tensor, $P(V)$, phonons	viscosity, thermal conductivity
nature	derivative of ground-state energy	transport, no energy functional
this route	**direct, no averaging**	**not reached**

Equilibrium continuum mechanics follows from RealQM by differentiating computed energies. Dissipation does not follow at all, and is the whole of what remains open (Section 6).

What is given up, stated plainly. The direct route delivers the *coefficients* of the macroscopic laws, not their *form*. Writing (3) presupposes that E is quadratic in the strain near equilibrium — that is, it assumes Hooke's law rather than deriving it. Homogenisation would instead produce linear elasticity as the macroscopic limit, form and coefficient together, and that is a genuine advantage of the formal route which should not be waved away.

Two things reduce the force of the objection. The form can be established computationally: compute $E(\epsilon)$ across a range and verify that it is quadratic, and that the departure from quadratic sets in where nonlinear elasticity is observed to set in. That is a demonstration and not a theorem. And a demonstration is the kind of evidence this programme is built to give — its standing claim is that its assertions are testable *because* computable, and reaching instead for an asymptotic theorem would borrow precisely the sort of authority it declines to grant to the standard formalism elsewhere. The formal route remains worth having; it is not what the next computation should wait for.

References

[1] Y. Deng, Z. Hani and X. Ma, *Hilbert's sixth problem: derivation of fluid equations via Boltzmann's kinetic theory*, arXiv:2503.01800 (2025).

[2] *Comment on "Hilbert's Sixth Problem: Derivation of Fluid Equations via Boltzmann's Kinetic Theory" by Deng, Hani and Ma*, arXiv:2504.06297 (2025).

[3] C. Johnson, *The Hydrodynamic Form of RealQM: Madelung Hydrostatics, a Surface Tension, and the Missing Half.*

[4] C. Johnson, *RealQM: Quantum Mechanics as Multiphase 3D Continuum Mechanics*, in [5].

[5] C. Johnson, *Real Quantum Mechanics* (Body&Soul, Vol. VI), https://claes542.github.io/RealMolecule/realquantum3.pdf.

[6] C. Johnson, *Conduction in RealQM: the Free Boundary as Charge Carrier*, in [5].

[7] C. Johnson, *Energy without Mass: the Kinetic Coefficient as a Geometric Scale, and Inertia as* E/c^2.

[8] C. Johnson, *Computational Thermodynamics* (Body&Soul, Vol. V).

[9] C. Johnson, *Upscaling of RealQM towards Hilbert's Sixth Problem*, companion paper.

[10] C. Johnson, *RealQM for Atoms and the Periodic Table.*

[11] C. Johnson, *The Clay Navier–Stokes Problem and Computational Well-Posedness.*