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QUANTUM COSMOLOGICAL METROLAND MODEL

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Abstract

Relational particle mechanics is useful for modelling whole-universe issues such as quantum cosmology or the problem of time in quantum gravity, including some aspects outside the reach of comparably complex minisuperspace models. In this article, we consider the mechanics of pure shape and not scale of 4 particles on a line, so that the only physically significant quantities are ratios of relative separations between the constituents' physical objects. Many of our ideas and workings extend to the N-particle case. As such models' configurations resemble depictions of metro lines in public transport maps, we term them 'N-stop metrolands'. This 4-stop model's configuration space is a 2-sphere, from which our metroland mechanics interpretation is via the 'cubic' tessellation. This model yields conserved quantities which are mathematically SO(3) objects like angular momenta but are physically relative dilational momenta (i.e. coordinates dotted with momenta). We provide and interpret various exact and approximate classical and quantum solutions for 4-stop metroland; from these results one can construct expectations and spreads of shape operators that admit interpretations as relative sizes and the 'homogeneity of the model universe's contents', and also objects of significance for the problem of time in quantum gravity (e.g. in the naïve Schrödinger and records theory timeless approaches).

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1 Introduction

Euclidean relational particle mechanics (ERPM) (proposed in [1] and further studied in [2, 3, 4, 5, 6, 7, 9, 10, 11, 12, 13]) is a mechanics in which only relative times, relative angles and relative separations are meaningful. On the other hand, in similarity relational particle mechanics (SRPM) (proposed in [15] and further studied in [16, 5, 17, 7, 18, 9, 19, 20, 13]), only relative times, relative angles and ratios of relative separations are meaningful. More precisely, these theories implement the following two Barbour-type relational¹ postulates.

- 1) They are *temporally relational* [1, 21, 22, 23, 18], i.e. there is no meaningful primary notion of time for the whole system thereby described (e.g. the universe), which is implemented by using actions that are manifestly reparametrization invariant while also being free of extraneous time-related variables [such as Newtonian time or General Relativity (GR)'s lapse]. This reparametrization invariance then directly produces primary constraints quadratic in the momenta.
- 2) They are *configurationally relational*, which can be conceived in terms of a certain group G of transformations that act on the theory's configuration space \mathbf{Q} being held to be physically meaningless [1, 21, 22, 23, 18, 13]. This can be implemented by such as using arbitrary- G -frame-corrected quantities rather than 'bare' \mathbf{Q} -configurations. For, despite this augmenting \mathbf{Q} to the principal bundle $P(\mathbf{Q}, G)$, variation with respect to each adjoined independent auxiliary G -variable produces a secondary constraint linear in the momenta which removes one G degree of freedom and one redundant degree of freedom among the \mathbf{Q} variables. Thus, one ends up dealing with the desired reduced configuration space – the quotient space \mathbf{Q}/G . Configurational relationalism includes as subcases both spatial relationalism (for spatial transformations) and internal relationalism (in the sense of gauge theory).

For ERPM, the Jacobi-type [24] action is²

$$I = 2 \int d\lambda \sqrt{T\{E - V\}}, \quad \text{with } T = \sum_i \mu_i \{\dot{\underline{R}}^i - \dot{\underline{b}} \times \underline{R}^i\}^2/2, \quad (1)$$

and for SRPM, our presentation of it is

$$I = 2 \int d\lambda \sqrt{T\{E - V\}}, \quad \text{with } T = \sum_i \mu_i \{\dot{\underline{R}}^i - \dot{\underline{b}} \times \underline{R}^i + \dot{c} \underline{R}^i\}^2/2I. \quad (2)$$

These implement the above relational postulates for the corresponding Euclidean and similarity G 's [1, 15, 6, 17, 9]. Equivalent theories formulated directly in terms of rotational (and dilational) invariant quantities can also be arrived at by considering the space of shapes and mechanics thereupon [30, 18]. It is then of interest what structure one gets when one quantizes such theories [26, 6, 8, 19, 10, 27, 11, 20, 12, 13, 14, 28].

The Barbour-type indirect formulation of RPM's (1,2), moreover, is particularly interesting through how the geometrodynamical form of GR can be cast in direct parallel: it also obeys postulates 1) and 2) implemented as follows [21, 23, 31] (some features of which are already anticipated in [32]).³

$$S^{\text{GR}} = 2 \int d\lambda \int d^3x \sqrt{h} \sqrt{T^{\text{GR}}\{\text{Ric}(h) - 2\Lambda\}} \quad \text{for } T^{\text{GR}} = \frac{1}{4} \mathcal{M}^{\mu\nu\rho\sigma} \{\dot{h}_{\mu\nu} - \mathcal{L}_{\dot{F}} h_{\mu\nu}\} \{\dot{h}_{\rho\sigma} - \mathcal{L}_{\dot{F}} h_{\rho\sigma}\}; \quad (3)$$

in this case, \mathbf{Q} is the space $\text{Riem}(\Sigma)$ of Riemannian 3-metrics on a fixed spatial topology Σ , and G is the corresponding 3-diffeomorphism group, $\text{Diff}(\Sigma)$.

The way that the physical equations follow from each of the above actions then has many parallels. By reparametrization invariance [34] each has a primary constraint quadratic in the momenta: for GR the Hamiltonian constraint

$$\mathcal{H} \equiv \mathcal{N}_{\mu\nu\rho\sigma} \pi^{\mu\nu} \pi^{\rho\sigma} - \sqrt{h} \{\text{Ric}(h) - 2\Lambda\} = 0 \quad (4)$$

¹RPM's are relational in Barbour's sense of the word rather than Rovelli's distinct one; see e.g. [59, 3, 4] for these authors' original material and [9] for a discussion of some differences.

² \underline{R}^i are relative Jacobi coordinates [25]: linear combinations of relative particle separation vectors that produce a diagonal kinetic term and are particular inter-particle cluster separation vectors with associated cluster masses μ_i . Lower-case Latin indices run over 1 to $n = N - 1$ for N the number of particles, and lower-case Greek ones are spatial indices; the spatial dimension is d . λ is label time and $\dot{}$ is the derivative with respect to this. Using such relative coordinates, one has already incorporated the highly trivial translation part of the Euclidean or similarity groups. $\dot{\underline{b}}$ is a rotational auxiliary velocity whereby the rotation part of these groups is implemented. In the SRPM case, \dot{c} is a dilational auxiliary velocity implementing the additional scaling part. $M_{i\alpha j\beta} = \mu_i \delta_{ij} \delta_{\alpha\beta}$ is the mass matrix with determinant M and inverse $N^{i\alpha j\beta}$. \underline{P}_i is the momentum conjugate to \underline{R}^i . I is the moment of inertia, $\sum_i \mu_i |\underline{R}^i|^2$. For ERPM, T , V and E are kinetic, potential and total energy terms with the usual physical dimensions. In our 'pure shape' formulation of the SRPM, the kinetic term T has dimensions of (energy)/ I and $E - V$ has dimensions of (energy) $\times I$. Consistency dictates that this V additionally be a homogeneous function of the \underline{R}^i ; in fact, in the given 'pure shape' formulation, it must be homogeneous of degree zero. This turns out not to be a heavy restriction due to I being constant after variation and useable to homogenize (see Sec 2 for an example). While an actual energy is prohibited by this consistency, the abovementioned constant E is permissible instead.

³The spatial topology Σ is taken to be compact without boundary. $h_{\mu\nu}$ is a spatial 3-metric thereupon, with determinant h , covariant derivative D_μ , Ricci scalar $\text{Ric}(h)$ and conjugate momentum $\pi^{\mu\nu}$. Λ is the cosmological constant. $\mathcal{M}^{\mu\nu\rho\sigma} = h^{\mu\rho} h^{\nu\sigma} - h^{\mu\nu} h^{\rho\sigma}$ is the inverse DeWitt supermetric with determinant \mathcal{M} and inverse $\mathcal{N}_{\mu\nu\rho\sigma}$. To represent this as a configuration space metric (i.e. with just two indices, and downstairs), use DeWitt's 2 index to 1 index map [33]. \dot{F}^μ is the velocity of the frame; in the manifestly relational formulation of GR, this cyclic velocity plays the role more usually played by the shift Lagrange multiplier coordinate. $\mathcal{L}_{\dot{F}}$ is the Lie derivative with respect to \dot{F}^μ .

and, for ERPM and SRPM respectively, the ‘energy constraints’:

$$\mathbb{Q} \equiv N^{i\alpha j\beta} P_{i\alpha} P_{j\beta} / 2 + V = E \quad , \quad \mathbb{Q} \equiv IN^{i\alpha j\beta} P_{i\alpha} P_{j\beta} / 2 + V = E \quad . \quad (5)$$

By variation with respect to the auxiliary G -variables, each relational theory has constraints linear in the momenta: for GR, the momentum constraint

$$\mathcal{L}_\mu \equiv -2D_\nu \pi^\nu_\mu = 0 \quad (6)$$

from variation with respect to F^μ , and, for RPM’s, the zero total angular momentum and zero total dilational momentum constraints

$$\underline{\mathbb{L}} \equiv \sum_i R^i \times \underline{P}_i = 0 \quad , \quad \mathbb{D} \equiv \sum_i R^i \cdot \underline{P}_i = 0 \quad (7)$$

from variation with respect to b^μ and c (so the latter constraint occurs only in SRPM). The zero total dilational momentum constraint moreover closely parallels the well-known GR maximal slicing condition [35], $h_{\mu\nu} \pi^{\mu\nu} = 0$. Furthermore, much like generalizing maximal slicing to constant mean curvature slicing [36] turns on a ‘York time’ variable [37, 38] $t^{\text{York}} \equiv \frac{2}{3} h_{\mu\nu} \pi^{\mu\nu} / \sqrt{h}$, one can think of the passage from SRPM to ERPM as involving an extra ‘Euler time’ variable $t^{\text{Euler}} \propto \sum_i R^i \cdot \underline{P}_i$. This is all underlied for both GR and RPM’s by shape-scale splits, the role of scale being played by \sqrt{I} or I for RPM’s and by such as the scalefactor a or \sqrt{h} in GR. In both cases it is then tempting to use the singled-out scale as a time variable but this runs into monotonicity problems which are avoided by using as times the quantities conjugate to (a function of) the scale, i.e. t^{York} and t^{Euler} .

There are further analogies at the configuration space level. If 1) $\text{R}(\mathbb{N}, d)$ the *relative space* of relative interparticle (cluster) separation vectors and $\text{Riem}(\Sigma)$ are held to be analogous, then so are 2) *Relational space* = $\text{R}(\mathbb{N}, d)/\text{Rot}(d)$ for $\text{Rot}(d)$ the d -dimensional rotations and superspace $(\Sigma) = \text{Riem}(\Sigma)/\text{Diff}(\Sigma)$. 3) *Shape space* = $\text{R}(\mathbb{N}, d)/\text{Rot} \times \text{Dil}$ for Dil the dilations and conformal superspace [39, 40] $\text{CS}(\Sigma) = \text{Riem}(\Sigma)/\text{Diff}(\Sigma) \times \text{Conf}(\Sigma)$ for $\text{Conf}(\Sigma)$ the conformal transformations on Σ . 4) The cone representation of relational space in shape-scale split variables [11] and $\{\text{CS} + \text{V}\}(\Sigma) = \text{Riem}(\Sigma)/\text{Diff}(\Sigma) \times \text{VPCConf}(\Sigma)$ [36] for $\text{VPCConf}(\Sigma)$ the conformal transformations that preserve the volume of the universe, V [41]. Also, both these GR and RPM configuration spaces are in general stratified, and both have physically significant bad points (e.g. $a = 0$ is the Big Bang and $I = 0$ is the maximal collision).

There are yet more analogies [42, 33, 37, 43, 44, 38, 3, 45, 46, 4, 47, 17, 48] at the level of various strategies toward the resolution of the Problem of Time⁴ and various other aspects of quantum cosmology. The above quadratic constraints give frozen (i.e. timeless or stationary) quantum equations. For GR, this is the Wheeler–DeWitt equation,

$$\widehat{\mathcal{H}}\Psi = -\hbar^2 \left\{ \frac{1}{\sqrt{\mathcal{M}}} \frac{\delta}{\delta h^{\mu\nu}} \left\{ \sqrt{\mathcal{M}} \mathcal{N}^{\mu\nu\rho\sigma} \frac{\delta\Psi}{\delta h^{\rho\sigma}} \right\} - \xi \text{Ric}(\mathcal{M})\Psi \right\} , \quad -\sqrt{h}(\text{Ric}(h) - 2\Lambda)\Psi = 0 \quad , \quad (8)$$

where Ψ is the wavefunction of the universe; ‘ \cdot ’ implies in general various well-definedness issues (see e.g. [19] for a summary) and need for a choice of operator-ordering (we use conformal ordering in this paper, c.f. Sec 3.1). Correspondingly, for RPM’s,

$$\widehat{\mathcal{Q}}\Psi = -\frac{\hbar^2}{2} \left\{ \frac{1}{\sqrt{M}} \frac{\partial}{\partial Q^A} \left\{ N^{AB} \sqrt{M} \frac{\partial}{\partial Q^B} \right\} - \xi \text{Ric}(M)\Psi \right\} \Psi + \text{V}\Psi = \text{E}\Psi \quad . \quad (9)$$

For the moment $A = i\alpha$, $B = j\beta$ and the Q^A are the $R^{i\alpha}$. N^{AB} is the inverse mass matrix for ERPM and I times it for SRPM. However, we use this equation more generally than that below for reduced RPM’s in which linear constraints have been taken care of, this being explicitly possible in 1- or 2- d [18].

An important feature of GR (and one missed out by minisuperspace models [49, 50]) is that of linear constraints causing substantial complications e.g. in attempted resolutions of the Problem of Time. That is the momentum constraint for GR [(6) or its quantum counterpart], while RPM’s have the linear constraints [(7) or their quantum counterparts]. However, minisuperspaces, unlike RPM’s, have more specific and GR-inherited potentials and indefinite kinetic terms. Thus both minisuperspace and RPM’s are valuable in complementary ways as toy models.⁵

Some of the strategies toward resolving the Problem of Time are as follows.

A) Perhaps one is to find a time hidden within classical GR [38] and thus obtain a wave equation that depends on it from the outset at the quantum level. York time is a GR example of such and Euler time is an ERPM model of it.

B) Perhaps one has slow, heavy ‘H’ variables that provide an approximate timestandard with respect to which the other fast, light ‘L’ degrees of freedom evolve [52, 38, 47]. In quantum cosmology the role of H is played by scale (and homogeneous matter modes), so ERPM’s in scale–shape split are more faithful semiclassical models of this than SRPM’s themselves can muster.

C) A number of approaches take timelessness at face value. One considers only questions about the universe ‘being’, rather than ‘becoming’, a certain way. This can cause at least some practical limitations, but nevertheless can address

⁴This notorious problem occurs because ‘time’ takes a different meaning in each of GR and ordinary quantum theory. This incompatibility underscores a number of problems with trying to replace these two branches with a single framework in situations in which the premises of both apply, namely in black holes and in the very early universe. While frozen quantum equations due to quadratic and not linear momentum dependence in the GR Hamiltonian constraint are one facet of the Problem of Time, this does have many other facets [38].

⁵Midisuperspace [51] unites all these desirable features but is unfortunately then computationally too hard for many of the strategies.

at least *some* questions of interest. For example, Hawking and Page’s *naïve Schrödinger interpretation* [53] concerns the ‘being’ probabilities for universe properties such as: what is the probability that the universe is large? Flat? Isotropic? Homogeneous? One obtains these via consideration of integrals of $|\Psi|^2$ over suitable regions of the configuration space. This approach is termed ‘naïve’ due to it not using any further features of the constraint equations. The *conditional probabilities interpretation* [43] goes further by addressing conditioned questions of ‘being’ such as ‘what is the probability that the universe is flat given that it is isotropic?’ *Records theory* [43, 55, 45, 4, 56, 57] involves localized subconfigurations of a single instant – whether these contain useable information, are correlated to each other, and whether a semblance of dynamics or history arises from this. RPM’s are superior to minisuperspace for such a study as they have a notion of localization in space, and more options for well-characterized localization in configuration space through their kinetic terms possessing positive-definite metrics.

D) Perhaps instead it is the histories that are primary (*histories theory* [55, 58]). There is a records theory within histories theory, and histories decohering is one possible way of obtaining a semiclassical regime in the first place, making B) to D) of particular interest to one of us [57, 10].

E) Distinct timeless approaches involve *evolving constants of the motion* (‘Heisenberg’ rather than ‘Schrödinger’ style QM), or *partial observables* [59] (which are used in loop quantum gravity’s *master constraint program* [60]).

Some approaches to the Problem of Time that do *not* have an RPM analogue include superspace time (which requires indefinite configuration spaces) and third quantization (which requires field theoretic rather than finite models).

We are in the process of building up a reasonable set of RPM models, paralleling e.g. the development of minisuperspace in the early 70’s [49, 50], or Carlip’s work in the 90’s for $2 + 1$ gravity [61] (see [38] for yet further useful toy model arenas for Problem of Time approaches). Also RPM’s serve as a bridge from highly-studied ideas in molecular physics and ‘mini- and midi’superspace, which may serve to import ideas and tools from the former to the latter.

Our build-up is for RPM’s in $1-d$ and $2-d$; for N particles, we term these, respectively, N -stop *metroland* and N -*agonland* (the first two nontrivial N -*agonlands* we furthermore refer to as *triangleland* and *quadrilateralland*). We choose to study these models because their configuration spaces are highly tractable mathematically [30, 18]: \mathbb{S}^{N-2} spheres in $1-d$ and $\mathbb{C}\mathbb{P}^{N-2}$ complex projective spaces in $2-d$. This is for the choice of plain shapes rather than oriented shapes. [I.e. we make the choice of treating each shape and its mirror image as distinct; in this paper’s 4-stop metroland model, this means that we regard the 1,2,3,4 ordering of the particles to be distinct from the 4,3,2,1 one. The opposite choice gives configuration spaces $\mathbb{S}^k/\mathbb{Z}_2 = \mathbb{R}\mathbb{P}^k$ (real projective spaces), and $\mathbb{C}\mathbb{P}^k/\mathbb{Z}_2$ which are somewhat harder to model.] N.B. that the interesting theoretical parallels between GR and RPM’s are unaffected by our choice of plain shapes and of low- d RPM’s. We are presently studying scalefree models as these are more straightforward than models with scale (though we will need to move on to scaled models as regards reasonably quantum-cosmologically realistic modelling of the semiclassical approach; note also that scalefree problems occur as a subproblems in models with scale [63, 18, 9], so studying these first also makes sense even from this semiclassical quantum cosmological perspective).

This paper considers scalefree 4-stop metroland (the smallest scalefree metroland to have the nontrivialities associated with having 2 physical degrees of freedom, so that one physical quantity can be expressed in terms of another, a feature necessary for records theory’s correlations, while semiclassical approaches need at least one H and at least one L, decoherence only makes sense if one thing decoheres another, and so on). Additionally, there are indications that 4-stop metroland is simpler than triangleland [11] (which also has two physical degrees of freedom and spherical shape space by $\mathbb{C}\mathbb{P}^1 = \mathbb{S}^2$), particularly in the cases with scale and at the quantum level, so that the present paper is useful toward how to subsequently deal with these other more complicated cases. Also, many of the present paper’s workings readily extend to N -stop metroland. 4-stop metroland and triangleland are both useful preliminaries for studying quadrilateralland, which is the simplest RPM to exhibit a number of geometrical nontrivialities, including some relevant to Problem of Time approaches and some that are archetypal of $2-d$ problems in ways that triangleland is not. Moreover, 4-stop metroland itself is already suitable for study of various timeless approaches to the Problem of Time.

In Sec 2 we consider a classical treatment of 4-stop metroland in its reduced form. We give a tessellation of the shape sphere corresponding to 4-stop metroland’s physical interpretation and provide useful and meaningful shape quantities for our study. We then study 4-stop metroland’s equations of motion and its conserved quantities, among which some have angular momentum-like mathematics but are physically dilational rather than angular momenta. We interpret simple subcases of multiple harmonic oscillator-like potentials’ solutions using our tessellation and shape quantities, concentrating on the case of two localized and well-separated subsystems that is motivated by our interest in timeless approaches.

In Sec 3 we consider time-independent Schrödinger equations for these problems, by firstly interpreting their exact and asymptotic solutions against our tessellation. Secondly, we compute expectations and spreads of our shape quantities promoted to quantum-mechanical shape operators. Thirdly, we consider perturbations about the simplest case in which the ‘springs’ balance each other out to produce a constant potential and hence spherical harmonics mathematics. Fourthly, we note and apply a number of analogies with molecular physics to our study. We conclude in Sec 4, including discussion of how our model and slightly larger versions thereof can be used as an arena for investigation of a number of Problem of Time strategies – of which we provide naïve Schrödinger interpretation examples – and by commenting on ‘mini- and midi’superspace counterparts of this paper’s shape operators.

2 4-stop metroland at the classical level

2.1 Passage to reduced form of 4-stop metroland and useful coordinatizations of it

The unreduced action is given by the SRPM case within eq. (2) further restricted to being in 1- d (so there are no rotations) and for 4 particles, and so 3 relative separations and thus 3 relative Jacobi coordinates, R^i :

$$I = 2 \int d\lambda \sqrt{T\{E - V\}} \quad \text{with} \quad T = \sum_{i=1}^3 \mu_i \{\dot{R}^i + \dot{c}R^i\}^2 / 2I. \quad (10)$$

We will find it more convenient to deal with the subsequent physics in terms of $\iota^i \equiv \sqrt{\mu_i}R^i$ the *mass-weighted* relative Jacobi coordinates [which are physically the square roots of the partial moments of inertia $I^i = \mu_i R^{i2}$ (no sum)], and, after variation, their ‘normalized’ counterparts $n^i = \iota^i/\iota$ and $N^i = I^i/I$ for I the total moment of inertia and $\iota = \sqrt{I}$. It will often be convenient to use n_x, n_y, n_z for the components of n^i . We take these Jacobi coordinates to be, in terms of particle position coordinates, Jacobi H-coordinates rather than Jacobi K-coordinates (Fig 1) with quantum cosmological and records theoretic applications in mind: two equal particle number clusters treated on the same footing, each could model the seed of a galaxy, or be a nontrivial record (of which we need at least 2 to consider correlations between records).

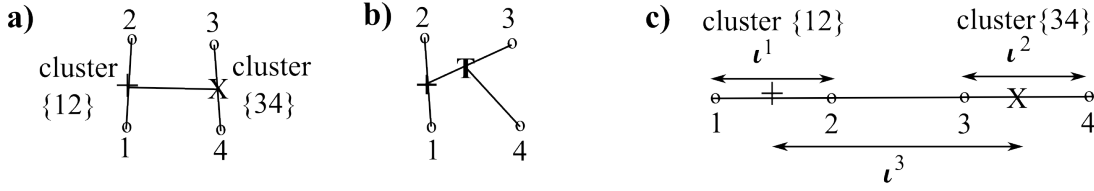


Figure 1: a) and b) explain in 2- d the origin of the names H- and K-coordinates. Using $\{a\dots c\}$ to denote the cluster composed of particles a, \dots, c ordered from left to right, $+$ is the centre of mass (COM) of cluster $\{12\}$, X is the COM of cluster $\{34\}$ and T is the COM of the triple cluster $\{123\}$. c) What H-coordinates look like in 1- d : the H has been ‘squashed’.

Now let us perform some variational manoeuvres on the above action. It is useful to bear in mind from the outset that our 4-stop metroland’s reduced configuration space is \mathbb{S}^2 and we are trying to bring this out as cleanly as possible by removing extraneous variables and seeking for standard coordinates on this. Variation with respect to the dilational auxiliary c gives the dilational constraint (7), the Lagrangian form for which can be rearranged to

$$\dot{c} = - \sum_{i=1}^3 \mu_i R^i \dot{R}^i / \sum_{j=1}^3 \mu_j \{R^j\}^2, \quad (11)$$

and used to eliminate \dot{c} from the action, producing (2) but with T_{red} in place of T :

$$T_{\text{red}} = \left\{ \sum_{i=1}^3 \{\iota^i\}^2 \sum_{j=1}^3 \{\iota^j\}^2 - \left\{ \sum_{i=1}^3 \iota^i \iota^i \right\}^2 \right\} / 2 \left\{ \sum_{k=1}^3 \{\iota^k\}^2 \right\}^2. \quad (12)$$

Then, via the coordinate transformation

$$\Theta = \arctan \left(\sqrt{\{\iota^1\}^2 + \{\iota^2\}^2} / \iota^3 \right), \quad \Phi = \arctan (\iota^2 / \iota^1), \quad (13)$$

(12) becomes

$$T_{\mathbb{S}^2} = \{\dot{\Theta}^2 + \sin^2 \Theta \dot{\Phi}^2\} / 2. \quad (14)$$

The coordinate ranges are $0 < \Theta < \pi$ and $0 \leq \Phi < 2\pi$, so these are geometrically the standard azimuthal and polar spherical angles on the unit shape space sphere \mathbb{S}^2 . Inversely,

$$\iota^1 = \iota \sin \Theta \cos \Phi, \quad \iota^2 = \iota \sin \Theta \sin \Phi, \quad \iota^3 = \iota \cos \Theta. \quad (15)$$

Thus 4-stop metroland has $\iota \equiv \sqrt{I}$ playing a (constant) radius role, and the ι^i are Cartesian coordinates in the ‘surrounding’ Euclidean relational space $R(4, 1) = \mathbb{R}^3$, subject to the on-sphere condition

$$\sum_{i=1}^3 I^i = \sum_{i=1}^3 \{\iota^i\}^2 = \{\iota\}^2 = I \quad (\text{constant}), \quad \text{or} \quad \sum_{i=1}^3 N^i = \sum_{i=1}^3 \{n^i\}^2 = 1. \quad (16)$$

The n^i are then the components of the unit Cartesian vector $[(\sin \Theta \cos \Phi, \sin \Theta \sin \Phi, \cos \Theta)]$ in spherical polar coordinates]. This should be contrasted with the way the sphere arising in scalefree triangleland [9] being harder to deal with from the perspective of the ‘surrounding’ Euclidean relational configuration space, which is \mathbb{R}^3 . Scalefree triangleland’s $\underline{\iota}^1$ and $\underline{\iota}^2$ are related to the Cartesian coordinates of the surrounding relational space not in the above familiar Cartesian way, but rather in the less straightforward ‘Dragt’ way [11], corresponding to having to use not ι but I as radial variable.

The following formulae are also useful below:

$$\cos \Theta = n_z, \quad \sin \Theta = \sqrt{n_x^2 + n_y^2}, \quad \cos \Phi = \frac{n_x}{\sqrt{n_x^2 + n_y^2}}, \quad \sin \Phi = \frac{n_y}{\sqrt{n_x^2 + n_y^2}}, \quad \cos 2\Phi = \frac{n_x^2 - n_y^2}{n_x^2 + n_y^2}, \quad \sin 2\Phi = \frac{2n_x n_y}{n_x^2 + n_y^2}, \quad (17)$$

and what is (from the geometrical perspective) a stereographic radial coordinate,

$$\mathcal{R} = \tan \frac{\Theta}{2} = \sqrt{\{1 - n_z\} / \{1 + n_z\}}. \quad (18)$$

2.2 Action and banal-conformal representations for this paper

We take the Jacobi action corresponding to (14),

$$I = 2 \int d\lambda \sqrt{T_{\mathbb{S}^2} \{E - V\}} \quad (19)$$

to be primary. As well as by Sec 2.1's reduction, this can be obtained by [18] considering a natural mechanics in Jacobi's geometrical sense [24] on the space of shapes [30].

The 'banal' conformal invariance of each of the above product-type actions $T \longrightarrow \Omega^2 T$, $E - V \longrightarrow \{E - V\}/\Omega^2$ is useful below in 'passing' factors between T and $E - V$ (which we term 'picking a distinct banal representation'). The above-given forms of T and $E - V$ are the geometrically-natural ones (both in the scale-invariant sense and in the sense of having the standard spherical metric on the shape space sphere) and mechanically-natural in the sense that E itself appears in them rather than E times some power of the moment of inertia. However, in some applications, (\mathcal{R}, Φ) coordinates and $\Omega = \{1 + \mathcal{R}^2\}/2$ is useful; we term this the 'flat banal representation' as its T is flat, and denote it by tilde-ing.

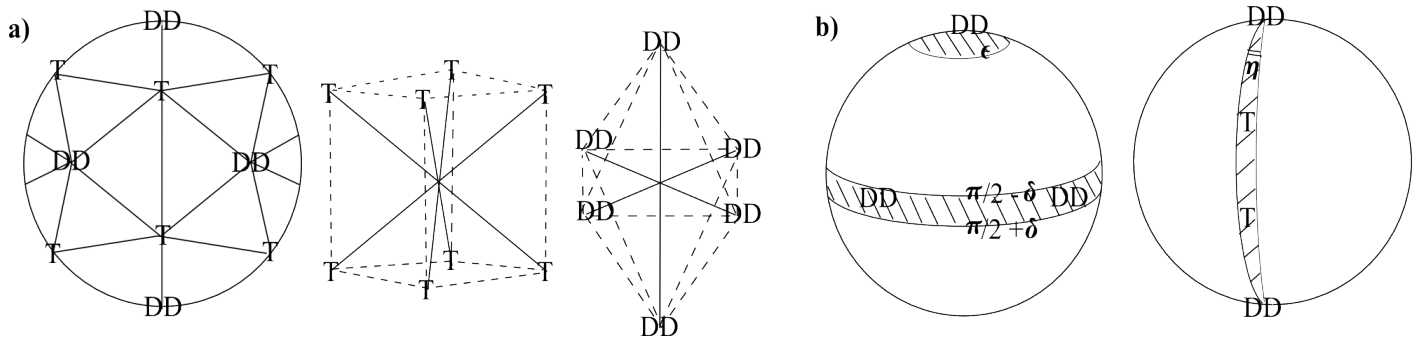


Figure 2: a) On the configuration space represented as a sphere, there are 8 triple collision (T) points and 6 double-double (DD) collision points. Each DD is attached to 4 T's, and each T to 3 T's and 3 DD's, in each case by single double collision lines. This forms a tessellation with 24 identical spherical isosceles triangle faces, 36 edges and 14 vertices. The T's and DD's form respectively the vertices of a cube and the octahedron dual to it (dashed lines in the second and third subfigures), so that the physical interpretation has the symmetry group of the cube, of order 48. This is isomorphic to $S_4 \times \mathbb{Z}_2$ for S_4 the permutation group of 4 objects, thus realizing the ways of labelling the 4 particles and ascribing an orientation. See pp. 72-75 of [64] for mathematical discussion of this tessellation and [65] for another occurrence of it in mechanics. In this arrangement, the T's and DD's form 7 antipodal pairs, thus picking out 7 preferred axes. The 3 axes corresponding to antipodal DD pairs are related to the 3 permutations of Jacobi H-coordinates and the 4 axes corresponding to antipodal T pairs are related to the 4 permutations of Jacobi K-coordinates. This relation is in the sense that the poles in each case correspond to what each coordinatization picks out as intra-cluster coordinates both going to zero i.e. collapse of both clusters for an H or collapse of the triple cluster for a K.

b) To make statements concerning shapes being near a DD or T - i.e. *well-localized* (intra-cluster distances far smaller than external distances to non-member particles/clusters), spherical caps $\Theta \leq \epsilon$ are useful in the corresponding spherical polar coordinate chart. In particular, with this paper's usual choice of axis, the polar caps are where there is both {12} and {34} localization, so following clusters {12} and {34} makes sense. Denote this clustering (i.e. partition into clusters) by {12,34}. The opposite notion is *merged clusters* for which the COM's of {12} and {34} are near each other so that these clusters largely overlap (which is, in a certain sense, a more 'homogeneous' universe model). This corresponds to belts $\pi/2 - \delta \leq \Theta \leq \pi/2 + \delta$ around the equator. (Multi)lunes $\Phi_0 - \eta \leq \Phi \leq \Phi_0 + \eta$ also correspond to physically meaningful statements. E.g. being in the bilune around the Greenwich meridian means that the {34} cluster is localized, being in the bilune around the 'Bangladeshi' meridian perpendicular to the Greenwich one means that the {12} cluster is localized and being in the tetralune at $\pi/4$ to all of these signifies that clusters {12} and {34} are of similar size', i.e. η -close to *contents homogeneity* (i.e. that the particle clusters that make up the model universe are, among themselves, of similar constitution). The above sort of approximate notions of shape are in the spirit of those used in e.g. Kendall et al. [30], and we make use of the corresponding configuration space regions in our naïve Schrödinger approach calculations in Sec 4.3. Moreover, note that notions of 'relative size' and 'similar contents' here in fact involve more concretely the $\sqrt{\text{mass} \times \text{distance}}$ combination (whose squares are partial moments of inertia).

2.3 Physical interpretation by tessellation, charts and shape operators

The Jacobi H-coordinates in use are better-adapted for 'seeing' double-double collisions [see Fig 2a)] rather than triple collisions (the opposite is the case for Jacobi K-coordinates), so that it is useful to preliminarily work out and graphically represent the mechanical interpretations of the various zones of our problem's configuration space of shapes: Fig 2. This is of considerable use below in interpreting classical trajectories (as paths upon this figure) and classical potentials and quantum-mechanical probability density functions (as height functions over this figure). Spherical polar coordinates about each axis in Fig 2 are natural for the study of the corresponding H or K structure. Thus each choice of H- or K-coordinates has a different natural spherical polar coordinate chart. Any two of these natural charts suffice to form an atlas for the sphere (each goes bad solely at its poles, where its axial angle ceases to be defined). To look extremely close to a pole, one can 'cartesianize' e.g. after projecting the relevant hemisphere onto the equatorial disc.

The n^i are interesting quantities with which to describe the shape of the configuration. Of course, only 2 of the 3 n^i are independent, by the on-sphere restriction (16). For the example of H-coordinates that follows the {12,34} clustering arrangement that we follow in particular in this paper, the corresponding n_z is a signed quantifier of the relative size of the universe from the perspective of an observer in either cluster. On the other hand, n_x is a signed quantifier of the size

of the universe from the less Copernican perspective of an observer specifically in cluster $\{12\}$ [n_y has the same meaning but for cluster $\{34\}$]. Thus we term these shape quantities $\text{RelSize}(12,34)$, $\text{RelSize}(1,2)$ and $\text{RelSize}(3,4)$ respectively.⁶

$\text{RelSize}(12,34)$ small means that clusters $\{12\}$ and $\{34\}$ are merged, and corresponds geometrically to the equatorial belt. $\text{RelSize}(12,34)$ large means physically that clusters $\{12\}$ and $\{34\}$ each cover but a small portion of the model universe, and corresponds geometrically to the polar caps. $\text{RelSize}(1,2)$ small means physically that cluster $\{12\}$ is but a speck in the firmament, and corresponds geometrically to a belt around the ‘Bangladeshi’ meridian. $\text{RelSize}(1,2)$ large means physically that cluster $\{12\}$ engulfs the rest of the model universe, and corresponds geometrically to an antipodal pair of caps around each of the intersections of the equator and the Greenwich meridian.

A quantifier of the contents inhomogeneity between the two clusters is Φ , which is related to the ratio of the size of $\{34\}$ to that of $\{12\}$ ’s by (13). N.B. that the last 3 paragraphs refer, more concretely, to $\sqrt{\text{mass}} \times \text{length}$, so that large mass hierarchies can distort intuitive notions of ‘actual size’.

2.4 Rotor and planar mechanics analogies for 4-stop metroland

By inspection of the kinetic term, there are clear analogies between this 4-stop metroland problem and well-known rotor and planar problems in ordinary mechanics. For the first analogy,

$$\arctan(\sqrt{\{\text{RelSize}(12)^2 + \text{RelSize}(34)^2\}}/\text{RelSize}(12,34)) = \Theta \longleftrightarrow \theta = (\text{azimuthal coordinate of the axis in space}) \quad (20)$$

$$\arctan(\text{RelSize}(34)/\text{RelSize}(12)) = \Phi \longleftrightarrow \phi = (\text{polar coordinate of the axis in space}) , \quad (21)$$

$$1 \leftrightarrow I_{\text{rotor}} \quad (\text{moment of inertia of the rotor}) . \quad (22)$$

For the second analogy, transform Θ to the radial stereographic coordinate $\mathcal{R} = \tan \frac{\Theta}{2}$ and pass to the ‘tilded’ banal representation. One then has the flat plane polar coordinates kinetic term, so

$$\sqrt{\{1 - \text{RelSize}(12, 34)\}/\{1 + \text{RelSize}(12, 34)\}} = \mathcal{R} \longleftrightarrow r = (\text{radial coordinate of test particle}) , \quad (23)$$

$$\arctan(\text{RelSize}(34)/\text{RelSize}(12)) = \Phi \longleftrightarrow \phi = (\text{polar coordinate of test particle}) , \quad (24)$$

$$1 \leftrightarrow m = (\text{test particle mass}) . \quad (25)$$

These analogies will be furtherly fruitful in analyzing 4-stop metroland’s equations of motion and conserved quantities in the next 2 subsections, as well as when further specifics about the potential are brought in (see Sec 3.6).

2.5 Equations of motion for 4-stop metroland

The equations of motion are

$$\Theta^{**} - \sin \Theta \cos \Theta \Phi^{*2} = -V_{,\Theta} , \quad \{\sin^2 \Theta \Phi^*\}^* = -V_{,\Phi} . \quad (26)$$

(The star is derivative with respect to the relational approach’s emergent time t : $* \equiv d/dt \equiv \sqrt{\{E - V\}/T}$; for which the equations of motion simplify. This is readily deduced to banal-transform as $* \longrightarrow \Omega^{-2}*$ [68].)

V is independent of λ itself and so one of these can be replaced by the ‘energy relation’ (a first integral):

$$\{\Theta^{*2} + \sin^2 \Theta \Phi^{*2}\}/2 + V(\Theta, \Phi) = E , \quad \text{constant} . \quad (27)$$

If the potential is additionally Φ -independent (which we term ‘special’ and whose planar mechanics analogue is termed central), then the Φ -Euler–Lagrange equation above gives another first integral,

$$\sin^2 \Theta \Phi^* = \mathcal{D} . \quad (28)$$

For both of the analogies above, the corresponding $\text{SO}(2)$ or $\text{SO}(3)$ related constant of the motion has the physical meaning of an angular momentum; for its interpretation in the present context, however, see the next subsection. In the special case, one can now furthermore combine the last 2 equations in two ways. Firstly,

$$E = \Theta^{*2}/2 + \mathcal{D}^2/2\sin^2 \Theta + V(\Theta) \equiv \Theta^{*2}/2 + V_{\text{eff}} \quad (29)$$

which in the planar central problem amounts to modification of the potential by a centrifugal barrier, while, in the more directly analogous rotor problem, amounts to placing a centrifugal barrier at each pole. In our problem, it takes the latter ‘bipolar barrier’ form. Secondly, (for $\mathcal{D} \neq 0$) $\Theta_{,\Phi}^2/2 = \sin^4 \Theta \{E - V_{\text{eff}}\}/\mathcal{D}^2$. Both of these straightforwardly give quadratures relating Θ to, respectively, t (orbit traversal rate) and Φ (shape of the orbit, the $\mathcal{D} = 0$ case giving a $\Phi = \text{constant}$ 1- d motion without any double barrier).

If V is also Θ -independent and thus constant, we get 3 \mathcal{D} -quantities from freedom to pick whichever axis to have a conserved Φ about. We call this constant-potential case the ‘very special case’ (the counterpart of which in the second analogy is the rigid rotor).

⁶There are other such operators corresponding to attaching significance to other clustering arrangements obtained by permuting the particles in defining the Jacobi H-coordinates, while similar quantities can be defined for the various permutations of Jacobi K-coordinates; see [20] for a brief account of the shape operators for each of these. $\text{RelSize}(12,34)$ is also $\sqrt{1 - n_x^2 - n_y^2}$, so it can also be viewed as a ‘measure’ of noncollapse of at least one of the model universe’s clusters; one can readily work out such ‘dual statements’ for other shape quantities.

2.6 Further discussion of 4-stop metroland's conserved quantities

One interesting issue in RPM's is what these angular momentum-like quantities are physically. Triangleland is spatially 2- d and as such affords a notion of angular momentum; its conserved quantity \mathcal{J} turns out to be the *relative* angular momentum between its subsystems. But the present paper's 4-stop metroland problem, however, is spatially 1- d , so no angular momentum in space (relative or otherwise) is possible. What then is the meaning of the conserved quantity \mathcal{D} in terms of the n^i or RelSize variables?

$$\mathcal{D} = n_x n_y^* - n_y n_x^* , \quad (30)$$

which is the '3-component of an angular momentum in the Euclidean relational configuration space $R(4,1) = \mathbb{R}^3$ '. Moreover, using \mathcal{D}_i for individual/partial dilations $R^i P_i$ (no sum)

$$\mathcal{D} = \mathcal{D}_2 n_x / n_y - \mathcal{D}_1 n_y / n_x \quad (31)$$

so that \mathcal{D} is a (weighted) *relative dilational quantity* corresponding to a particular exchange of dilational momentum between the {12} and {34} clusters.

In the very special case, there are 3 \mathcal{D} conserved quantities forming a vector in the 'surrounding' Euclidean relational configuration space \mathbb{R}^3 , of which the above \mathcal{D} is the 3-component:

$$\mathcal{D}_i = \epsilon_{ijk} n^j n^{k*} = \mathcal{D}_k n^j / n^k - \mathcal{D}_j n^k / n^j \quad (32)$$

where i, j, k are a cycle of 1, 2, 3.

All in all, the less special a problem is, the more types of relative dilational momentum exchanges it has.

That we get 'angular momentum mathematics', we explain as follows. The body of mathematics habitually associated with angular momentum can actually be associated more generally (in terms of what physics it covers, not what mathematics it is, as further explained in Appendix A) with rational (i.e. 'ratio-based') quantities rather than just with angular ones (which are a subset thereof).⁷ Therefore 'rational momentum mathematics' would appear to be a more widely appropriate term, covering both angular momentum and dilational momentum as subcases. The objects in question continue to possess antisymmetry in this more general setting since this derives from differentiating a (function of a) ratio by the (chain rule and) quotient rule: $\{f(y/x)\}^* = f'\{xy^* - yx^*\}/x^2$ and thus occurs irrespective of whether that ratio admits an interpretation as an angle in physical space.

2.7 Passage to 4-stop metroland's Hamiltonian

The conjugate momenta are then

$$p_\Theta = \Theta^* , \quad p_\Phi = \sin^2 \Theta \Phi^* = \mathcal{D} . \quad (33)$$

[Also, $\mathcal{D}_i = \epsilon_{ij}{}^k \iota^j p_k$ for p_k the momentum conjugate to ι^k .] The momenta obey a quadratic constraint

$$\mathcal{Q} \equiv p_\Theta^2 / 2 + p_\Phi^2 / 2 \sin^2 \Theta + V(\Theta, \Phi) = E , \quad (34)$$

the middle expression of which also serves as the classical Hamiltonian \mathbf{H} for the system.

2.8 Harmonic oscillator like potentials for 4-stop metroland

With eventual timeless records and structure formation goals in mind, we intend to follow a particular clustering – the {12,34} one – using a particular permutation of H-coordinates which is physically picked out by considering not the most general array of 6 springs between the particles but rather the following. We take the mechanical picture in Jacobi coordinates as primary and consider springs within each of the {12} and {34} clusters and between the centres of mass of the two clusters (reinterpretable if one so wishes as a superposition of inter-particle springs). Then the potential is

$$\begin{aligned} V &= \sum_{i=1}^3 K_i \{n^i\}^2 / 2 = \{K_1^2 \sin^2 \Theta \cos^2 \Phi + K_2^2 \sin^2 \Theta \cos^2 \Phi + K_3^2 \cos^2 \Theta\} / 2 = \\ &A + B \cos 2\Theta + C \sin^2 \Theta \cos 2\Phi = a + b Y_{2,0}(\Theta) + c Y_{2,2c}(\Theta, \Phi) \end{aligned} \quad (35)$$

for $K_i = H_i / \mu_i$ where H_i play the role of Jacobi–Hooke coefficients, and

$$A = K_3 / 4 + \{K_1 + K_2\} / 8 , \quad B = K_3 / 4 - \{K_1 + K_2\} / 8 , \quad C = \{K_1 - K_2\} / 4 , \quad (36)$$

the Y 's are spherical harmonics (c and s subscripts thereon standing for cosine and sine Φ -parts) and the precise form of the constants a, b, c is not required for this paper. This potential has as a 'very special' case $B = C = 0$, for which the potential is constant, and the 'special case' $C = 0$ for which the dynamics is separable (which is sketched in Fig 3). In terms of the K_i , the special case corresponds to $K_1 = K_2$, i.e. that each cluster has the same 'constitution': the same Jacobi–Hooke coefficient per Jacobi cluster mass, which is a kind of 'homogeneity requirement' on the 'structure formation' in the cosmological analogy. The very special case then corresponds to $K_1 = K_2 = K_3$, for which high-symmetry situation

⁷Smith [62] pointed out this generalization but not, as far as we are aware of, its rational interpretation.

the various potentials can balance out to produce the constant. Additionally the $B \ll A$ perturbative regime about the very special case signifies $K_1 + K_2 \ll K_3$ so the inter-cluster spring is a lot stronger than the intra-cluster springs, which in some ways is analogous to scalefactor dominance over inhomogeneous dynamics in cosmology. On the other hand, the $C \ll A$ regime corresponds to either or both of the conditions $K_1 + K_2 \ll K_3$, $K_1 \approx K_2$ the latter of which signifies high contents homogeneity. The multiplicity of forms of writing the potential above is useful to bear in mind in searching for mathematical analogues for the present problem in e.g. the molecular physics literature (c.f. Sec 3.6).

If one started instead with springs between all 6 pairs of particles, one would obtain $V_6 = V + V'$ for

$$V' = \sum_{i=1}^3 L_i n^j n^k = D \sin^2 \Theta \sin 2\Phi + E \sin 2\Theta \cos \Phi + F \sin 2\Theta \sin \Phi = dY_{2,2s}(\Theta, \Phi) + eY_{2,1c}(\Theta, \Phi) + fY_{2,1s}(\Theta, \Phi) \quad (37)$$

where i, j, k are a cycle so that the first form of V_6 is the most general homogeneous quadratic polynomial in the n^i , $D = L_3/2$, $E = L_2/2$ and $F = L_1/2$, and the detailed form of the constants d, e and f are not needed for this paper. On the face of it, this is a more general problem than the preceding paragraph's, with three further nonseparable terms. However, there is a sense in which these three terms can be made to go away, c.f. Sec 2.12. One can imagine whichever of these problems' potentials as a superposition of familiar 'orbital shaped' lumps, though such a superposition will of course in general alter the number, size and position of peaks and valleys according to what coefficients each harmonic contribution has. Contrast with the triangleland model is also interesting at this point – there $Y_{0,0}$ and just two of the first-order spherical harmonics arose.

The equations of motion for this potential are

$$\Theta^{**} - \sin \Theta \cos \Theta \Phi^{*2} = \sin 2\Theta \{2B - C \cos 2\Phi - D \sin 2\Phi\} + 2 \cos 2\Theta \{E \cos \Phi + F \sin \Phi\}, \quad (38)$$

$$\{\sin^2 \Theta \Phi^*\}^* = 2 \sin^2 \Theta \{C \sin 2\Phi - D \cos 2\Phi\} + \sin 2\Theta \{E \sin \Phi - F \cos \Phi\}, \quad (39)$$

one of which can be replaced by the 'energy' first integral

$$\{\Theta^{*2} + \sin^2 \Theta \Phi^{*2}\}/2 + A + B \cos 2\Theta + C \sin^2 \Theta \cos 2\Phi + D \sin^2 \Theta \sin 2\Phi + E \sin 2\Theta \cos \Phi + F \sin 2\Theta \sin \Phi = E. \quad (40)$$

Then if $C = D = E = F = 0$, one has a special potential, so the Φ Euler-Lagrange equation gives another first integral (28) and the subsequent quadrature for the shape of the orbit is

$$\Phi - \Phi_0 = \pm D \int d\Theta / \sin \Theta \sqrt{2\{E - A - B \cos 2\Theta\} \sin^2 \Theta - D^2}. \quad (41)$$

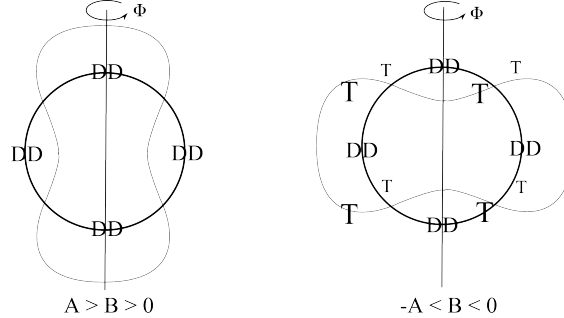


Figure 3: We sketch V over the sphere for the mechanically significant cases a) $A > B > 0$ and b) $-A < B < 0$. The first has barriers at the poles and a well around the equator, while the second has wells at the pole and a barrier around the equator. Each is a surface of revolution of the curve provided, the first case being a peanut or ellipsoid-like surfaces and the second case being a concave or convex wheel. In each case, considering V_{eff} for $D \neq 0$ adds a spike at each pole (this now means that for $D \neq 0$ both islands cannot simultaneously collapse to their generally distinct centre of mass points). Finally, note that our potential is axisymmetric and reflectible about its equator so its symmetry group is $\mathbb{D}_\infty \times \mathbb{Z}_2$ (\mathbb{D} denotes dihaedral). If this is aligned with a DD axis of the physical interpretation, the overall problem retains a $\mathbb{D}_4 \times \mathbb{Z}_2$ symmetry group, of order 16.

One simple consideration here is small and large regimes for the special case. More precisely, these are near-North Pole and near-South Pole regimes in Θ but become large and small regimes in terms of $\mathcal{R} = \tan \frac{\Theta}{2}$. For this (including changing to the tilded banal representation), and using 'shifted energy' $E' \equiv E - A - B$

$$W \equiv \tilde{E} - \tilde{V} = 4E' / \{1 + \mathcal{R}^2\}^2 + 32B\mathcal{R}^2 / \{1 + \mathcal{R}^2\}^4. \quad (42)$$

Then the near-North Pole regime ($\mathcal{R} \ll 1$) maps to the problem with flat polar kinetic term and

$$W = 4E' + 8\{4B - E'\}\mathcal{R}^2 \quad (43)$$

up to $O(\mathcal{R}^4)$. This has the mathematics of a 2- d isotropic harmonic oscillator,

$$W = \mathcal{E} - \omega^2 \mathcal{R}^2 / 2, \quad (44)$$

provided that the ‘classical frequency’ (for us with units of I/time) $\omega < 0$ (else it would be a constant potential problem or an upside-down harmonic oscillator problem), alongside $\mathcal{E} > 0$ to stand a chance of then meeting classical energy requirements. Writing \mathcal{E} and ω^2 out by comparing the previous two equations, these inequalities signify that $2E > K_3$ and $2E > K_3 + 2\{K_3 - K_1\}$, the latter being more stringent if $K_3 > K_1$ (‘stronger inter-cluster binding’) and less stringent if $K_3 \leq K_1$ (‘weaker inter-cluster binding’). One can also deduce from the first of these and $K_3 \geq 0$ (spring) that $E > 0$.

Next, note that the near-South Pole regime ($\mathcal{R} \ll 1$) maps to the problem with flat polar kinetic term and

$$W = 4E'/\mathcal{R}^4 + 8\{4B - E'\}/\mathcal{R}^6 \quad (45)$$

up to $O(1/\mathcal{R}^8)$. Moreover, $\mathcal{U} = 1/\mathcal{R}$ maps the large case’s (42) to the small case’s (45), so this is also an isotropic harmonic oscillator – in (\mathcal{U}, Φ) coordinates and with the same \mathcal{E} and ω as above. One of us had previously observed a ‘large–small’ duality of this sort in triangleland [9]. It halves the required solving to understand $\Theta \approx 0$ and $\approx \pi$. Another lesson learnt from the triangleland study is that we know that study of *second* approximations is considerably more profitable than that of first approximations, so we pass straight to them. Note that, for our subsequent QM study, we want the isotropic harmonic oscillator rather than cases corresponding to other values of the parameters \mathcal{E} and $-\omega^2$ (e.g. the upside-down isotropic harmonic oscillator).

2.9 Classical solutions for $\mathcal{D} = 0$

$0 = \mathcal{D} = \sin^2 \Theta \Phi^*$, so either $\sin \Theta = 0$ and one is stuck on a pole or Φ is constant. In terms of the n^i , this translates to $n_y = kn_x$ for k constant, so motion is restricted to lying on a diameter. In the case of $\mathcal{D} = 0$ (which corresponds to constant potential case with $\mathcal{D} = 0$), one likewise obtains $n_y = kn_x = ln_z$ for l also constant, but (16) holds too, so all n^i take fixed values and motion is restricted to a point. Being purely 1- d or 0- d motions, this subsection’s solutions’ simpleness renders them of limited interest. 1- d motions include 1) going up and down the 1-axis, corresponding to cluster {34} always being collapsed while cluster {12} varies in size including going through zero size at the origin and two triple collisions in which each of particles 1 and 2 coincide with the collapsed cluster. 2) The {12} \leftrightarrow {34} of this going up and down the 2-axis. 3) Going up and down an $n_y = \pm n_x$ line, corresponding to the clusters always being of the same size (contents homogeneity) but that size varying from zero ({12,34} DD collision, i.e. {12} collapsing to a point and also {34} collapsing to a point) to maximal [in which the two clusters are superposed into the {13,24} or {14,23} DD collisions].

2.10 Classical solution in the very special case

For $\mathcal{D} \neq 0$, the very special case is solved by the geodesics on the shape space sphere,

$$\cos(\Phi - \Phi_0) = \kappa \cot \Theta \quad (46)$$

for $\kappa = \mathcal{D}/\sqrt{2\{E - A\} - \mathcal{D}^2}$, constant. Then in terms of the n^i (or RelSize variables), (17 i-iv) gives

$$\kappa n_z = n_x \cos \Phi_0 + n_y \sin \Phi_0, \quad (47)$$

i.e. restriction to a plane through the origin, with arbitrary normal $(\cos \Phi_0, \sin \Phi_0, -\kappa)$. But also $\sum_{i=1}^3 \{n^i\}^2 = 1$, so we are restricted to the intersection of the sphere and the arbitrary plane through its centre, which is clearly another well-known way of describing the great circles as circles within \mathbb{R}^3 .

The disc in the equatorial plane is particularly useful for considering the mechanics of the problem with clusters {12} and {34} picked out by our choice of Jacobi H-coordinates. Eliminating n_z projects an ellipse onto this disc,

$$\kappa^2 = \{\kappa^2 + \cos^2 \Phi_0\} n_x^2 + 2 \cos \Phi_0 \sin \Phi_0 n_x n_y + \{\kappa^2 + \sin^2 \Phi_0\} n_y^2, \quad (48)$$

centred on the origin with its principal axes in general not aligned with the coordinates. E.g. for $\Phi_0 = 0$, the ellipse is

$$\{\text{RelSize}(1,2)/\{1 + \kappa^{-2}\}^{-1/2}\}^2 + \text{RelSize}(3,4)^2 = 1, \quad (49)$$

which has major axis in the $\text{RelSize}(3,4) = n_y$ direction and minor axis in the $\text{RelSize}(1,2) = n_x$ direction, while the value of $\text{RelSize}(12,34) = n_z$ around the actual curve can then be read off (47) to be $n_z = n_x/\kappa$. With reference to the first subfigure in Figure 2a), as $\mathcal{D} \rightarrow \infty$, the dynamical trajectory is the equator, corresponding to maximally-merged configurations including four DD collisions. For \mathcal{D} small, the motion approximately goes up and down a meridian, e.g. forming a basic unit of a narrow cycle from the polar DD to slightly around the T on the Greenwich meridian (reflections of) which is repeated various times to form the whole trajectory. [The actual limiting on-axis motion $\mathcal{D} = 0$ is excluded from this subsection’s working but already considered in the preceding one.]

Other Φ_0 straightforwardly correspond to rotated ellipses. However the mechanical meaning of these differs. E.g. about $\pi/2$ clusters {12} and {34} are interchanged, while about $\pm\pi/4$ also has distinct sharp physical significance. Throughout, note the periodicity of the motion (already clear in the spherical model as the great circles are closed curves). The tessellation’s edge-lines are great circles, projecting to the disc rim, the axes, the lines at $\pi/4$ to the axes and ellipses with principal directions aligned with the preceding.

2.11 Approximate classical solutions in the special case

At the level of the sphere and using the second approximation, we can transcribe the solution from [9] to be, with \mathcal{D} for \mathcal{J} and with our \mathcal{E} and ω^2 in place of that paper's Q_0 and Q_2 , and defining $f_0 = 2\mathcal{E}/\mathcal{D}^2$, $f_2 = \omega^2/\mathcal{D}^2$ and $g = \sqrt{f_0^2 - f_2}$,

$$\sqrt{f_0 + g \cos(2\{\Phi - \Phi_0\})} = 1/\mathcal{R} = \cot \frac{\Theta}{2}. \quad (50)$$

In terms of \mathcal{R} these are ellipses centred on the origin (including the bounding case of circles but excluding the other bounded case of pairs of straight lines (Fig 4).

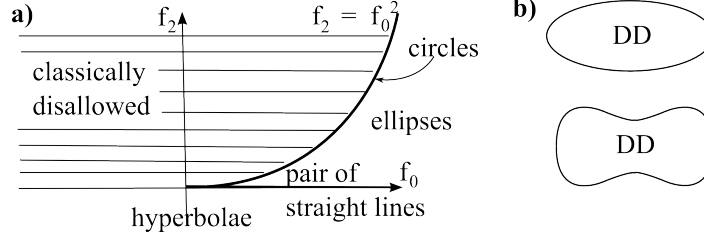


Figure 4: a) For the small approximation in (\mathcal{R}, Φ) coordinates, the desired parameter space is the indicated wedge populated by ellipses; on the bounding parabola, we get circles, coinciding with the edge of the n_x, n_y disc for $f_0 = 1 = f_2$ and becoming smaller in either direction. b) For the large approximation in (\mathcal{W}, Φ) coordinates, the parameter space is likewise; if one converts to (\mathcal{R}, Φ) coordinates, however, the wedge is then populated by ellipse-like curves and peanut-like curves.

N.B. we now have a third inequality on \mathcal{E} and ω : $4\mathcal{E}^2 \geq \mathcal{D}^2\omega^2$, that replaces $\mathcal{E} > 0$ as it is more stringent. Thus in terms of \mathbf{E} and the K_i we get our allowed wedge of parameter space to be $2\{2\mathbf{E} - K_3\}^2/\mathcal{D}^2 \geq \{2\mathbf{E} - K_3\} + 2\{K_1 - K_3\} > 0$. Saturation of this corresponds to circular trajectories. For such circles to exist, the discriminant gives the condition $\{\mathcal{D}/4\}^2 \geq K_3 - K_1$, so that the relative dilational quantity is bounded from below by the amount by which the inter-cluster spring dominates.

Then by (17 v-vi) and (18), (50) becomes

$$\sqrt{f_0 + g\{(n_x^2 - n_y^2) \cos 2\Phi_0 + 2n_x n_y \sin 2\Phi_0\}/\{n_x^2 + n_y^2\}} = \sqrt{\{1 + n_z\}/\{1 - n_z\}}, \quad (51)$$

so solving for n_z and applying the on-sphere condition for $\Phi_0 = 0$, say, gives

$$\sqrt{1 - n_x^2 - n_y^2} = n_z = \frac{\{f_0 + g - 1\}n_x^2 + \{f_0 - g - 1\}n_y^2}{\{f_0 + g + 1\}n_x^2 + \{f_0 - g + 1\}n_y^2}. \quad (52)$$

Then one can write down a curve in terms of two independent variables such as $\text{RelSize}(1,2)$ and $\text{RelSize}(3,4)$: either $\text{RelSize}(1,2) + \text{RelSize}(3,4) = 0$ (so both are 0 because they are positive and so both clusters have collapsed) or

$$\{\{f_0 + g + 1\}\text{RelSize}(1,2)^2 + \{f_0 - g + 1\}\text{RelSize}(3,4)^2\}^2 = 4\{\{f_0 + g\}\text{RelSize}(1,2)^2 + \{f_0 - g\}\text{RelSize}(3,4)^2\}. \quad (53)$$

The large regime then has

$$\sqrt{f_0 + g \cos(2\{\Phi - \Phi_0\})} = 1/\mathcal{W} = \mathcal{R} = \tan \frac{\Theta}{2}, \quad (54)$$

which is, for the cases of interest, an ellipse-like or peanut-like curve (see [9] and Fig 4b). Applying this paper's interpretation in terms of n^i or RelSize variables, the *same* answer as for the small regime arises again. This conclusion just reflects the potential imposed having an antipodal symmetry, which physically translates to shapes and their mirror images behaving in the same fashion.

Finally, note that this approximate problem has a part-hidden $\text{SO}(3)$ symmetry (such are well-known for harmonic oscillators). In the present context, however, its objects take the form

$$\mathcal{H}_1 = \omega n_x n_y + \mathcal{D}_1 \mathcal{D}_2 / \omega n_x n_y, \quad \mathcal{H}_2 = \mathcal{D} = \mathcal{D}_2 n_x / n_y - \mathcal{D}_1 n_y / n_x, \quad \mathcal{H}_3 = \omega \{n_x^2 - n_y^2\} / 2 + \mathcal{D}_1^2 / 2\omega n_x^2 - \mathcal{D}_2^2 / 2\omega n_y^2. \quad (55)$$

Thus its unhidden part is $\mathcal{H}_2 = \mathcal{D}$ which has relative dilational momentum significance, while its remaining hidden parts are mixed shape and dilational objects. [This is used as an example in Appendix A.]

2.12 Discussion of 'more general combinations of springs'

The L_i terms (or, equivalently, D , E and F terms) can be dropped in the sense that one can pass to normal coordinates for which the symmetric matrix of Jacobi-Hooke coefficients has been diagonalized. Unlike in triangle-land, however, this does not send one to the special case – the C -term survives and so requires addressing separately (e.g. perturbatively). The elimination thus of D , E and F terms is also subject to the mechanical interpretation of the normal-coordinate problem being more difficult algebraically than for $D = E = F = 0$, so that it is conceivable that one might prefer to retain this simpler interpretation and treat D , E and F perturbatively.

3 4-stop metroland at the quantum level

Kinematical quantization [66] for this problem [19] involves three objects u^i whose squares add up to 1 (which in the present case we identify with the Cartesian unit vectors n^i) and three SO(3) objects (which in the present case are the \mathcal{D}_i). We then consider the time-independent Schrödinger equation [19]

$$\{\sin \Theta\}^{-1}\{\sin \Theta \Psi_{,\Theta}\}_{,\Theta} + \{\sin \Theta\}^{-2}\Psi_{,\Phi\Phi} = \{A + B \cos 2\Theta + C \sin^2 \Theta \cos 2\Phi\}\Psi, \quad (56)$$

where $A = 2\{A - E\}/\hbar^2$, $B = 2B/\hbar^2$, $C = 2C/\hbar^2$ are dimensionless constants. Note that the above equation is separable for $0 = C$ i.e. $0 = C$ i.e. $K_1 = K_2$; most of our work is for this case.

3.1 Explanation of the choice of operator ordering

We choose an ordering that is coordinatization invariant on configuration space [67], i.e. a member of the family $D^2 - \xi \text{Ric}(M)$ [c.f. (8, 9)] where D^2 and $\text{Ric}(M)$ are the Laplacian and the Ricci scalar corresponding to the kinetic metric M on configuration space. Moreover, following from the appropriateness of relational actions for whole-universe physics, observing that these have banal conformal invariance as a simple and natural feature and then asking for this to hold at the quantum level in the whole-universe context (i.e. in quantum cosmology or toy models thereof), among the preceding family of orderings we are uniquely led to the *conformal ordering*, for which $\xi = \{k - 2\}/4\{k - 1\}$, where k is the configuration space dimension. (See [68] for more on this motivation for conformal ordering, previous motivation on different premises for it being in e.g. [49, 69].) Moreover, presently we are in configuration space dimension 2, for which $\xi = 0$ so our operator ordering choice is, in this case the same as the Laplacian ordering (itself advocated in e.g. [70], while [71] also considered $2-d$ configuration spaces so the Laplacian–conformal ordering coincidence also applies).

3.2 Solution in very special case

The $C = 0$ case of Eq (56) separates to simple harmonic motion and the Θ equation

$$\{\sin \Theta\}^{-1}\{\sin \Theta \Psi_{,\Theta}\}_{,\Theta} - \{\sin \Theta\}^{-2}m^2\Psi = \mathcal{A}\Psi + B \cos 2\Theta \Psi, \quad (57)$$

If $B = 0$ as well – our very special problem –, then from Sec 2.4 this has similar mathematics to ordinary QM’s central potential problem, in which the quantum Hamiltonian \hat{H} , total angular momentum $\hat{L}_{\text{Total}} = \sum_{\alpha=1}^3 \hat{L}_{\alpha}^2$ and magnetic/axial/projected angular momentum \hat{L}_3 form a complete set of commuting operators and as such share eigenvalues and eigenfunctions. In fact (also Sec 2.4) our very special problem is mathematically the same as the rigid rotor, for which \hat{H} is L_{Total} up to multiplicative and additive constants, so, effectively one has a complete set of two commuting operators, whose eigenvalues and eigenfunctions are the well-known spherical harmonics and, moreover also occur as a separated-out part of the corresponding scaled relational particle model problem. However, our ‘rigid rotor’ is in configuration space rather than in space and with total relative dilational momentum $\hat{D}_{\text{Total}} = \sum_{i=1}^3 \hat{D}_i^2$ in place of total angular momentum and projected relative dilational momentum \hat{D}_3 in place of axial angular momentum. These then have eigenvalues $\hbar^2 D\{D + 1\}$ and $\hbar d$ respectively, so we term D and d respectively the *total* and *projected relative dilational quantum numbers* (in analogy with the rigid rotor).

Our very special problem’s time-independent Schrödinger equation separates into simple harmonic motion and the associated Legendre equation (in $X = \cos \Theta$) i.e. the spherical harmonics equations, Thus its solutions are

$$\Psi_{Dd}(\Theta, \Phi) \propto Y_{Dd}(\Theta, \Phi) \propto P_D^d(\cos \Theta) \exp(\pm id\Phi) \quad (58)$$

for $P_D^d(X)$ the associated Legendre functions of X , $D \in \mathbb{N}_0$ and d such that $|d| \leq D$. Also, $D\{D + 1\} = -\mathcal{A}$, which, interpreted in terms of the original quantities of the problem, is the condition

$$E' = E - K_3/2 = \hbar^2 D\{D + 1\}/2 \quad (59)$$

on the model universe’s ‘energy’ and inter-cluster effective spring in order to have any quantum solutions (E is fixed as this is a whole-universe model so there is nothing external from which it could gain or lose energy). If this is the case, there are then $2D + 1$ solutions labelled by d (we can see the preceding sentence cuts down on a given system’s solution space, though the more usual larger solution space still exists in the ‘multiverse’ sense [20]).

Furthermore, using a basis with sines and cosines instead of positive and negative exponentials,

$$\Psi_{D\mathcal{N}}(n^i) \propto \mathcal{N}(n^i). \quad (60)$$

Here, the D -label runs over the orbital types (s for $D = 0$, p for $D = 1$, d for $D = 2$...) and \mathcal{N} is the ‘naming polynomial’ i.e. 1 for s , n_x for p_{n_x} , $n_x n_y$ for $d_{n_x n_y}$ etc. (Note that the name ‘ z^2 ’ in $d_{n_x z}$ is indeed *shorthand* for $z^2 - 1/3$; shorthand begins to proliferate if one goes beyond the d -orbitals; the polynomials arising in our working are also subject to being ‘nonunique’ under $\sum_{i=1}^3 \{n^i\}^2 = 1$.) That the wavefunctions are their own naming polynomials is via Sec 2.4’s analogy 2

mirroring how the orbitals in space historically got their Cartesian names, and also is akin to representations [72] of the spherical harmonics in terms of homogeneous polynomials. Another form for the solution is⁸

$$\Psi_{D|d|}(n^i) \propto P_D^d(n_z) \mathcal{T}_d \left(n_x / \sqrt{n_x^2 + n_y^2} \right) = P_D^d(\text{RelSize}(12,34)) \mathcal{T}_d \left(\text{RelSize}(1,2) / \sqrt{1 - \text{RelSize}(12,34)^2} \right). \quad (61)$$

However, via Sec 2.3's tessellation trick, we can interpret the wavefunctions in terms of the metroland mechanics on the sphere itself, on which they take the particularly familiar 'orbital' form.

For $D, d = 0, 0$ (s -orbital), note that the axis is arbitrary so it is evident from using 2 different principal axes that the probability distribution function on-axis is not to be trusted in spherical coordinates about that axis. We conclude that the ground state does not have bias toward any particular configurations. For $D, d = 1, 0$ (p_{n_z} orbital), equatorial configurations are improbable, meaning that mergers of the {12} and {34} clusters [including the non {12,34} DD's] are disfavoured, while polar configurations are probable, meaning that the {12} and {34} clusters being small and well-apart is favoured. For $D, d = 1, \pm 1$, in the p_{n_y} orbital case, the $n_y = \text{RelSize}(3,4)$ axis part of the equator is probable, so mergers of a small {12} and a large {34} are favoured. p_{n_x} is the {12} \leftrightarrow {34} of this. For $D, d = 2, 0$ ($d_{n_z^2}$ orbital), both equatorial and polar configurations are probable, so that the {12} and {34} clusters are either merged or small and well-apart. For $D, d = 2, \pm 1$, in the $p_{n_y n_z}$ case, equatorial configurations are improbable, so mergers of {12} and {34} are improbable, and also the {12} cluster is small; DD's are disfavoured. $d_{n_x n_z}$ is the {12} \leftrightarrow {34} of this. For $D, d = 2, \pm 2$, in the $d_{n_x^2 - n_y^2}$ case, equatorial configurations, i.e. mergers of {12} and {34}, are probable, especially those with one but not both of the clusters are large (i.e. configurations along one of the RelSize (12) or RelSize(34) axes: contents inhomogeneity), including the {13,24}, {14,23}, {23,14} and {24,13} DD's. In the $d_{n_x n_y}$ case, again equatorial configurations are probable, but now with $|\text{RelSize}(12)| \approx |\text{RelSize}(3,4)|$ i.e. contents homogeneity, including the DD's where the two clusters are on top of each other [{13,24} and {14,23}].

3.3 Overlap integrals: shapes and spreads of shape operators

We are interested furthermore in computing overlap integrals $\langle D_1 d_1 | \widehat{\text{Operator}} | D_2 d_2 \rangle$ for three applications 1) expectation and spread of shape operators (below). 2) Time-independent perturbation theory about the very special solution in Sec 3.5. 3) Time-dependent perturbation theory on space of shapes with respect to a time provided by the scale in the shape-scale split ERPM models in semiclassical formulation also makes use of these. This parallels Halliwell–Hawking's work [52] and embodies one of our program's eventual goals, so we prefer giving details of computing the overlaps to giving details of 2). 2) and 3) have the merit of extending to far more general potential terms than the harmonic oscillator-like terms discussed in the present working, while 2) survives as a subproblem in the corresponding time-independent non-semiclassically approximated shape-scale split ERPM.

The idea to use 1) such can be traced back to how expectations and spreads of powers of r are used in the study of atoms (see e.g. [73, 79] for elementary use in the study of hydrogen, or [74] for use in approximate studies of larger atoms). Doing this amounts to acknowledging that 'modal' quantities (peaks and valleys), as read off from plots or by the calculus, are only part of the picture: such as the mean $\langle n l m | r | n l m \rangle$, $\langle n l m | r^2 | n l m \rangle$ and the spread $\Delta_{n l m}(r) = \sqrt{\langle n l m | r^2 | n l m \rangle - \langle n l m | r | n l m \rangle^2}$ are also useful. E.g. for hydrogen, one obtains from the angular factors of the integrals trivially cancelling and orthogonality and recurrence relation properties of Laguerre polynomials in Appendix B for the radial factors that

$$\langle n l m | r | n l m \rangle = \{3n^2 - l(l+1)\}a/2 \quad \text{and} \quad \Delta_{n l m} r = \sqrt{\{n^2\{n^2 + 2\} - \{l(l+1)\}^2\}a/2}, \quad (62)$$

where a is the Bohr radius. One can then infer from this that a minimal typical size is $3a/2$ and that the radius and its spread both become large for large quantum numbers. c.f. how the modal estimate of minimal typical size is a itself; the slight disagreement between these is some indication of the limited accuracy to which either estimate should be trusted. Also, we identify the above as expectations of scale operators, and thereby next ask whether they have pure shape counterparts in the standard atomic context.

The answer is yes. Up to normalization, they are the 3- Y integrals [75] (for Y spherical harmonics, the radial parts of the integration now trivially cancelling), and the general case of this has been evaluated in terms of Wigner 3j symbols [75]. Furthermore, many of the integrals for the present paper's specific cases of interest are written out case-by case in [76] (this applies to expectations of the RelSize's as well as B, C, D, E, F perturbation terms' constituent overlaps). Shape operators for hydrogen are also considered in [77] (briefly) and [78].

Moreover, the context in which shape operators occur in molecular physics is wider than just the above. E.g. 1) expectations of $\cos \beta$ for β a relative angle from inner products between physically meaningful vectors e.g. between the 2 electron–nucleus relative position vectors in Helium, in the characterization of molecules' bonds or in nuclear spin-spin coupling (p 443 of [77]).

E.g. 2) one also gets expectations of $Y_{20}(\theta)$ [c.f. form 4 of (35)] in spin-spin and hyperfine interactions (p 437-441) of [77] (as a shape factor occurring alongside a $1/r^3$ scale factor.

⁸This is found by shifting from arctan to arccos and then using one of the standard definitions of Tchebychev polynomials, $T_d(\xi) = \cos(d \arccos(\xi))$ Despite being the product of two generally nonpolynomial factors, the two conspire to produce polynomials in each case. We then introduce the symbol $\mathcal{T}_d(\xi)$ to mean $T_d(\xi)$ for cosine solutions and $\sqrt{1 - T_d(\xi)^2}$ for sine solutions.

E.g. 3) In the study of the H_2^+ molecular ion, one uses fixed nuclear separation as a scale setter and then one has not only 1 relative angle but also 2 ratios forming spheroidal coordinates with respect to which this problem separates, and expectations of all these things then make good sense.

We contemplate ‘mini- and midi-’superspace counterparts of such shape operators in Sec 4.5.

As regards good shape operators for 4-stop metroland, the kinematical quantization carries guarantees that the three n^i are promoted to good quantum operators. These can be interpreted as RelSize(1,2), RelSize(3,4) and RelSize(12,34) as per Sec 2.3. It is also useful to note at this stage that n_z is not only physically RelSize(12,34) but also mathematically the Legendre variable.

Then $\langle D d | \widehat{\text{RelSize}}(1,2) | D d \rangle = \langle D d | \widehat{\text{RelSize}}(3,4) | D d \rangle = 0$ and $\langle D d | \widehat{\Theta} | D d \rangle \approx \langle D d | \widehat{\text{RelSize}}(12,34) | D d \rangle = 0$ as an obvious result of orientational symmetry. The useful information starts with the spreads,

$$\Delta_{D d}(\widehat{\text{RelSize}}(1,2)) = \sqrt{\frac{D\{D+1\} + d^2 - 1}{\{2D-1\}\{2D+3\}}} Q_1(d) \quad , \quad \Delta_{D d}(\widehat{\text{RelSize}}(3,4)) = \sqrt{\frac{D\{D+1\} + d^2 - 1}{\{2D-1\}\{2D+3\}}} Q_2(d) \quad , \quad (63)$$

$$\Delta_{D d}(\widehat{\Theta}) \approx \Delta_{D d}(\widehat{\text{RelSize}}(12,34)) = \sqrt{\frac{2\{D\{D+1\} - d^2\} - 1}{\{2D-1\}\{2D+3\}}} \quad , \quad (64)$$

for $Q_2(d) = 1/2$ for the d cosine solution, $3/2$ for the d sine solution, and 1 otherwise, and $Q_1(d)$ the $\sin \leftrightarrow \cos$ of this. One can then readily check that $\langle \widehat{n}_x^2 + \widehat{n}_y^2 + \widehat{n}_z^2 \rangle = 1$, as it should be.

One case of interest is the ground state. Therein, the spreads in each are $1/\sqrt{3}$. Another case of interest is the large quantum number limit. $\Delta_{D d}(\widehat{\Theta}) \approx \Delta_{D d}(\widehat{\text{RelSize}}(12,34))$ which, for the maximal d ($|d| = D$), is equal to $1/\sqrt{2D+3}$ which goes as $1/\sqrt{2D} \rightarrow 0$ for D large. The hydrogen counterpart of this result is $\Delta_{11}\widehat{\theta} \approx 1/\sqrt{2l} \rightarrow 0$, i.e. restriction to the Kepler–Coulomb plane (e.g. [77] outlines this, while [78] considers it in more detail). Back to our problem, this result therefore signifies recovery of the equatorial classical geodesic as the limit of an ever-thinner belt in the limit of large maximal projectional relative dilational quantum number $|d| = D$ (‘the rim of the disc’ of Sec 2.10, traversed in either direction according to the sign of d). In fact, as for the constant potential we can put the axis wherever we please, this leads to recovery of *any* of the classical geodesics. Also, for $d = 0$, $\Delta_{D 0}\widehat{\Theta} \approx \Delta_{D 0}(\widehat{\text{RelSize}}(12,34)) \rightarrow 1/\sqrt{2}$ for D large. This means that the $s, p_{n_z}, d_{n_z^2} \dots$ sequence of orbitals does not get much narrower as D increases, so that for these states we only get limited peaking about clusters $\{12\}$ and $\{34\}$ both being small and well apart, a situation which we will revisit in the next subsection due to its centrality to the assumptions made in, and applications of, this paper. The RelSize(1,2) and RelSize(3,4) operators’ spreads tend to finite constant values for large D no matter what value d takes.

What of $\widehat{\Phi}$? Now, clearly, by factorization and cancellation of the Θ -integrals, the $d = 0$ states obey the uniform distribution over 0 to 2π , with mean π and variance $\pi^2/3$ (corresponding to axisymmetry). Furthermore, $\langle D d | \widehat{\Phi} | D d \rangle$ is also π and cosine and sine states have

$$\Delta_{D d}(\widehat{\Phi}) = \sqrt{\pi^2/3 + 1/2d^2} \quad \text{and} \quad \Delta_{D d}(\widehat{\Phi}) = \sqrt{\pi^2/3 - 1/2d^2} \quad , \quad (65)$$

which indicate some resemblance to the uniform distribution arising for large d (mean and variance do not see the multimodality, but at least, by inspection along the lines of the preceding subsection, it is *regular* multimodality for d maximal – equatorial flowers of $2D$ petals – by inspection of the shapes of the standard maximal $s, p, d, f, g \dots$ orbitals.

3.4 Solution in special case – large and small regimes

Passing to stereographic coordinates, banal-conformal transforming to the flat representation and applying the small approximation, our Schrödinger equation becomes

$$-\{\hbar^2/2\}\{\mathcal{R}^{-1}\{\mathcal{R}\Psi_{,\mathcal{R}}\}_{,\mathcal{R}} + \mathcal{R}^{-2}\Psi_{,\Phi\Phi}\} = \mathcal{E} - \omega^2\mathcal{R}^2/2 \quad , \quad (66)$$

which is in direct correspondence with the $2-d$ quantum isotropic harmonic oscillator (see e.g. [73, 79, 80] under $\mathcal{R} \longleftrightarrow r$ (radial coordinate), $1 \longleftrightarrow$ particle mass, and with our ω as classical frequency ($\times I$). Thereby,

$$\mathcal{E} = \mathfrak{n}\hbar\omega \quad \text{for} \quad \mathfrak{n} \equiv 1 + 2N + |d| \quad (67)$$

for N a node-counting quantum number running over \mathbb{N}_0 and d a ‘projected’ dilational quantum number as in the preceding subsection but now running over \mathbb{Z} . [The ‘shifted energy’ in its usual units, $E' = E - A - B$, itself goes as

$$E' = \{\mathfrak{n}^2\hbar^2/2\}\{1 + \sqrt{1 - B\{4/\mathfrak{n}\hbar\}^2}\} \quad , \quad (68)$$

so for $\mathfrak{n}\hbar/\omega \ll 1$ (small quantum numbers as used below), $E'I \approx \mathfrak{n}\hbar\Omega$ for $\Omega = 2\sqrt{-B}$.] The solutions are then (to suitable approximation)

$$\Psi_{\text{Nd}}(\Theta, \Phi) \propto \Theta^{|d|}\{1 + |d|\Theta^2/12\}\exp(-\omega\Theta^2/8\hbar)L_N^{|d|}(\omega\Theta^2/4\hbar)\exp(\pm id\Phi) \quad (69)$$

for $L_a^b(\xi)$ the associated Laguerre polynomials in ξ (see Appendix B). [The Φ -factor of this is rewriteable as before in terms of the n^i or $\text{RelSize}(12,34)$ and $\text{RelSize}(1,2)$, while the Θ -factor is now a somewhat more complicated function of $\text{RelSize}(12,34)$].

The large regime gives the same eigenvalue condition (67), and (69) again for wavefunctions except that one now uses the supplementary angle $\Xi = \pi - \Theta$ in place of Θ . Next, see Fig 5 for the form and interpretation of the wavefunctions.

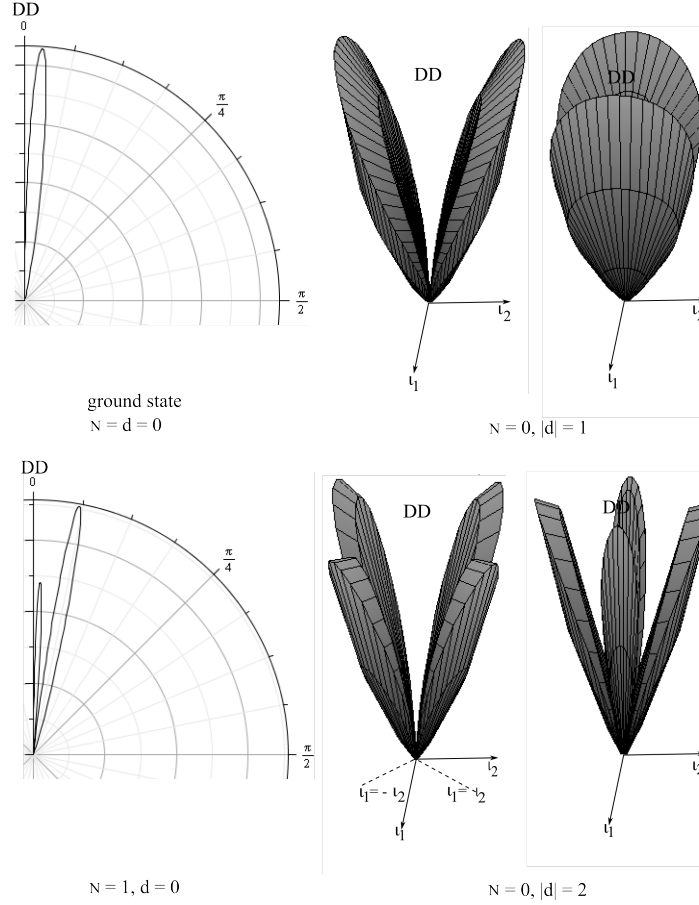


Figure 5: Probability density functions for this subsection's problem for ω/\hbar large, 400, say, plotted using Maple [81]. All $d = 0$ states are axisymmetric about the $\{12,34\}$ clustering's DD axis, i.e. all relative sizes for cluster $\{12\}$ and for cluster $\{34\}$ are equally favoured. The ground state is peaked around the $\{12,34\}$ DD collision. It is the surface of revolution of the given curve. The $N = 0, |d| = 1$ solutions are a degenerate pair. Each takes the form of a pair of inclined lobes – the cosine solution's oriented about the $n_x = \text{RelSize}(1,2) = 0$ D collision and the sine solution's about the $n_y = \text{RelSize}(3,4) = 0$ D collision. These next three solutions form a degenerate triplet. The $N = 1, d = 0$ solution is a slender bulge around the $\{12,34\}$ DD collision, then a gap and then a second bulge in the form of a cone, representing 'a band very close to this DD collision and a band somewhat close to it being probable, while all other configurations are improbable. The $N = 0, |d| = 2$ solutions are tulips of four petals, the cosine one separately favouring the lunes of near $\{12\}$ D collisions and near $\{34\}$ D collisions (i.e. contents inhomogeneity), while the sine one disfavours these and favours instead the lunes at $\pi/4$ to the preceding, which correspond to contents homogeneity of the $\{12\}$ and $\{34\}$ clusters. The large case's approximate solution is just the reflection of the preceding about the equatorial plane with the same interpretation except that $\{34\}$ is now to the left of $\{12\}$.

In the small regime, the $\text{RelSize}(1,2)$ and $\text{RelSize}(3,4)$ operators still have zero expectation as each sign for these remains equally probable. For D, d substantially smaller than ω/\hbar so powers of the latter dominate powers of the former (and ω/\hbar was considered to be large, so this works for the kind of quantum numbers in this subsection's specific calculations), the following mean and spread results for shape operators are derived using orthogonality of, and a recurrence relation for, Laguerre polynomials, as provided in Appendix B.

$$\langle N d | \widehat{\text{RelSize}}(12,34) | N d \rangle = 1 - 2n\hbar/\omega . \quad (70)$$

$\Delta_{N d} \widehat{\text{RelSize}}(12,34)$ is zero to first two orders, beyond which the approximations used begin to break down, but it would appear to have leading term proportional to \hbar/ω . These results signify that the potential has trapped what was much more uniform in Sec 3.3 into a narrow area around the $\{12,34\}$ DD collision. Furthermore,

$$\Delta_{N d} \widehat{n}^{\bar{a}} \approx \sqrt{2n\hbar Q_{\bar{a}}(d)/\omega} \quad (71)$$

for $\bar{a} = 1, 2$ gives $\Delta_{N d}(\widehat{\text{RelSize}}(1,2))$ for $\bar{a} = 1$ and $\Delta_{N d}(\widehat{\text{RelSize}}(3,4))$ for $\bar{a} = 2$. So one can obtain strong concentration around the poles by suitable choice of springs, amounting to a tall thick equatorial barrier and polar wells. The ground

state has the tightest spread in RelSize(1,2) and RelSize(3,4): $\sqrt{2\hbar/\omega}$. This has some parallels with how the Bohr radius is an indicator of atomic size, including the hydrogen-isotropic harmonic oscillator correspondence [79].

3.5 Perturbations about the very special solution

We begin by recasting our Schrödinger equation in Legendre variables $n_z = \cos \Theta$,

$$\{\{1 - n_z^2\}\Psi_{,n_z}\}_{,n_z} + \{1 - n_z^2\}^{-1}\Psi_{,\Phi\Phi} = \{A - B + n_z^2\{2B - C\cos 2\Phi\} + C\cos 2\Phi\}\Psi. \quad (72)$$

One can then study this using time-independent perturbation theory (see e.g. [75] for derivation of the formulae for this up to second order). Applying perturbation theory here means considering 1) C small, which is high contents homogeneity at the level of each cluster's (Hooke coefficient)/(reduced mass) in the sense that $K_1 - K_2$ is small compared to \hbar^2 . 2) B small, in the sense that \hbar^2 is large compared to $\{K_1 + K_2\}/2 - K_3$, which collapses to $K_1 - K_3$ small in the case of $C = 0$, meaning that there is little difference between the inter-cluster spring and the intra-cluster springs.

Perturbative study of (72) is amenable to exact calculations though involving various of trigonometric and standard/tabulated associated Legendre function integrals, or, alternatively, the aforementioned 3-Y integrals. Furthermore, this continues to be the case if one includes a non-diagonal/non-normal basis' D , E and F terms.

For the B -perturbation, as both it and the unperturbed Hamiltonian commute with \mathcal{D} , the eigenvalue problem can be solved separately in each subspace \mathcal{V}_d of a given eigenvalue d of \mathcal{D} , and in each such subspace the spectrum of the unperturbed Hamiltonian is nondegenerate, so that nondegenerate perturbation theory is applicable (this argument parallels e.g. p 697 of [73]). This gives (with the unperturbed problem's \mathcal{A} playing the role usually ascribed to the energy and H_1 the perturbative term) $\mathcal{A}_{D,d}^{(1)} = \langle Dd | H_1 | Dd \rangle$ at first order and $\mathcal{A}_{D,d}^{(2)} = -\sum_{D',d' \neq D,d} |\langle D'd' | H_1 | Dd \rangle|^2 / \{\mathcal{A}_{D'} - \mathcal{A}_D\}$ at second order [75]. Then e.g. [19] double use of a standard recurrence relation [82] gives a $\Delta d = 0$, $\Delta D = 0, \pm 2$ 'selection rule'. Moreover, the terms that survive this take the following forms.

$$\langle Dd | \mathcal{B}\{2n_z^2 - 1\} | Dd \rangle = \mathcal{B}\{1 - 4d^2\}/\{2D - 1\}\{2D + 3\}, \quad (73)$$

which is closely related to the expectation of $n_z = \text{RelSize}(12,34)$ already computed in Sec 3.3. Two new overlaps that are more general than expectations are

$$\langle D + 2d | \mathcal{B}\{2n_z^2 - 1\} | Dd \rangle = \frac{2\mathcal{B}}{2D + 3} \sqrt{\frac{\{\{D + 2\}^2 - d^2\}\{\{D + 1\}^2 - d^2\}}{\{2D + 5\}\{2D + 1\}}}, \quad (74)$$

and then, swapping D for $D - 2$, also,

$$\langle D - 2d | \mathcal{B}\{2n_z^2 - 1\} | Dd \rangle = \frac{2\mathcal{B}}{2D - 1} \sqrt{\frac{\{\{D^2 - d^2\}\{\{D - 1\}^2 - d^2\}}{\{2D + 1\}\{2D - 3\}}}. \quad (75)$$

Using these then gives the perturbed 'energies':

$$\begin{aligned} E_{D,d} = & A + \hbar^2 D\{D + 1\}/2 + B\{1 - 4d^2\}/\{2D - 1\}\{2D + 3\} + \\ & \frac{4B^2\{\{2D + 5\}\{2D + 3\}^3\{D^2 - d^2\}\{\{D - 1\}^2 - d^2\} - \{2D - 1\}^3\{2D - 3\}\{\{D + 2\}^2 - d^2\}\{\{D + 1\}^2 - d^2\}\}}{\hbar^2\{2D + 5\}\{2D + 3\}^3\{2D + 1\}\{2D - 1\}^3\{2D - 3\}} + O(B^3). \end{aligned} \quad (76)$$

Note that d positive and negative are treated the same, so there is only a partial uplifting of degeneracy. Changes to the wavefunction due to the perturbations for the sign of B corresponding to Sec 3.4 and to second order in B are that we get slight bulges at the poles for the ground state (a bit of $d_{n_z^2}$ mixed in).

The C perturbation can likewise be studied based on half-way stage overlaps that can be directly transcribed by our angular momentum to dilational momentum analogy from those computed in e.g. [76]. E.g. the surviving terms are found [19] by a second standard recurrence relation [82] to obey the selection rule $\Delta d = \pm 2$, $\Delta D = 0$. Some noteworthy features of the study of the C term are that degenerate perturbation theory is now required, there is no first order contribution as $\Delta d = \pm 2$ only, and now d and $-d$ do get shifted differently corresponding to this perturbation not preserving the axis of symmetry. In nondiagonal/nonnormal form, the further D term has the same selection rule to the C term's while the E and F terms share the selection rule $\Delta d = \pm 1$, $\Delta D = 0, \pm 2$. The above 'noteworthy features' apply to these also.

3.6 Molecular physics analogies

Analogy A) (57) occurs in mathematical physics (e.g. from the separation of the wave equation in prolate spherical coordinates [83, 84, 85, 82]) and has multiple applications in molecular physics studies of which parallel some of the studies in the present paper. Examples of this in molecular physics are as follows.

Analogy A.1) (57) recast in terms of the Legendre variable is

$$\{\{1 - n_z^2\}\Psi_{,n_z}\}_{,n_z} - \{1 - n_z^2\}^{-1}d^2\Psi = \{A - B + 2Bn_z^2\}\Psi, \quad (77)$$

which is the simpler of the two spheroidal equations that arise in the study of the H_2^+ molecular ion [86, 87, 88]. This and the next two analogies are for $B < 0$, although the aforementioned mathematical physics literature covers $B > 0$. Analogy A.2) The potential $V_0\{1 - \cos 2\theta\}$ [c.f. form 3 of (35)] occurs in modelling the rotation of a linear molecule in a crystal [90, 91, 89]. Here, the analogy is (21,20,22) where the axis and rotor in question are provided by the linear molecule itself, ‘energy’ \leftrightarrow energy up to a constant,

$$K_1/2 \leftrightarrow 2V_0 \text{ up to the same constant difference as in the energy analogy} \quad (78)$$

$$B \leftrightarrow -2V_0 \quad (79)$$

Analogy A.3) The potential $-\alpha_{||}\mathbf{E}^2 \cos^2\theta$ [c.f. form 2 of (35)] for $\alpha_{||}$ the polarizability along the axis occurs in the study [92, 93] of e.g. the CO_2 molecule in a background electric field \mathbf{E} (the study of polarizability is the theory underlying Raman spectroscopy). Here the analogy is, rather,

$$B \longleftrightarrow -\alpha_{||}\mathbf{E}^2/2. \quad (80)$$

Analogy A.4) Examples 2) of Sec 3.3 is another substantially developed area in the molecular physics literature.

Analogy B) is with the ammonia molecule NH_3 , in the following rougher but qualitatively valuable sense. NH_3 has two potential wells separated by a barrier and then is capable of tunnelling between the two at the quantum level (like an umbrella inverting in the wind). Our model for $B < 0$ is similar to this, albeit in spherical polar coordinates: we have 2 polar wells with an equatorial barrier in between.

This analogy then gives us some idea about how the separate solutions for the two wells compose. For NH_3 , one can start with separate solutions for each well and additional degeneracies ensue (due to the wells being identical and being able to distribute some fixed energies between these in diverse ways). However the wavefunctions tend to perturb each other toward breaking these degeneracies, forming symmetric and antisymmetric wavefunctions over the two wells [77, 87].

3.7 Applications of the analogies and developing an overall picture of our model

Firstly, the $B < 0$ locally stable small or large regimes are the kind of regimes that are termed ‘rotator-like’ in analogy A.2)’s literature; both of the SO(3) quantum numbers (for us, dilational quantum numbers) hold good in this regime.

Secondly, for $B < 0$ one can use Analogy B to form a simple picture of putting the small and large Θ approximations together. As d remains a good quantum number for the unapproximated problem, one expects to need the North Pole approximation’s d and the South Pole approximation’s d to match and the subsequent perturbations exacted by these two approximations upon each other not to affect d . Also, prior to any recombination, one has degeneracies as follows (call the near-North Pole’s node-counting quantum number N and the near-South Pole’s N'). There is the one ground state $N = N' = d = 0$, then the degenerate pair $N = N' = 0, d = \pm 1$, and then the degenerate quadruplet $N = 1, N' = 0$ or $N = 0, N' = 1$ for each of $d = \pm 1$. Now if N and N' match, expectation of $\text{RelSize}(12,34)$ goes to 0 again though the wavefunction’s distribution is bimodal about both poles. If they do not match, $\text{RelSize}(12,34)$ retains some nonzero expectation due to the peaking near the two poles being different in detail. The flip here, as in NH_3 , is an inversion, i.e. it reverses the orientation, sending 1,2,3,4 to 4,3,2,1.

Thirdly, analogy A.3) is well-known for its Raman-type ± 2 and not ± 1 selection rule, which parallels our results of Sec 3.5. Analogy A.3) has furthermore been studied perturbatively for what for us is the small $B < 0$ regime. This allows us to e.g. check the half-way house results (73, 74, 75) against pp. 271-273 of [93].

Fourthly, further resources from analogy A.1)’s references [84, 85] include analysis of this equation’s poles in the complex plane and how it admits a solution in the form of an infinite series in associated Legendre functions in the vicinity of ± 1 and in Bessel functions in the vicinity of ∞ , as well as how to piece together these different representations. It is then appropriate to compare results from the expansion in associated Legendre functions against our perturbative regime (this particular working holds regardless of the sign of B). Thus we find the lowest four cases of (76) to agree with pp. 1502-4 of [85], which additionally provides the corresponding wavefunctions which we use to first order in B in Sec 4.4 to evaluate the naïve Schrödinger interpretation probabilities for these states’ model universes being large.

Fifthly, one cannot really put together our near-polar calculations and our perturbative calculations, because the “ B small perturbative condition” goes a long way toward ω being small and then only a bit of the wavefunction is near the pole. Our near-polar calculations should be compared, rather, with the asymptotics for B large. Analogy A.2)’s literature covers this for what for us is the B large negative ($\gg E - A - B = E'$) regime, giving, via the analogy,

$$E' \sim N\hbar\omega_{\text{large}} + O(1/\omega_{\text{large}}) \text{ and} \quad (81)$$

$$\Psi \propto \exp(\omega_{\text{large}}\cos\Theta/\hbar) \left\{ \tan\frac{\Theta}{2} \right\}^{2N} \left\{ \sec\frac{\Theta}{2} \right\}^{2\{|d|+1\}} + O(1/\omega_{\text{large}}) \quad (82)$$

as the relevant asymptotic solutions, for $\omega_{\text{large}} = 2\sqrt{-B}$. Now, from (43,44) the small- Θ approximate solution (69)’s $\omega = 8\sqrt{-B} = 4\omega_{\text{large}}$, so $\exp(\omega_{\text{large}}\cos\Theta/\hbar)$ in (81) $\approx \text{const} \times \exp(\{\omega/4\hbar\}\{-\Theta^2/2\})$, which is indeed in agreement with the leading and dominant factor of (69). For our model, this regime signifies that $K_3 \gg K_1, K_2$ i.e. that the inter-cluster spring is much stronger than each of the intra-cluster springs. This is termed a ‘harmonic oscillator-like regime’

– comparing (81) and the standard result for the 2- d isotropic harmonic oscillator makes it clear why. d alone remains a good dilational quantum number in this regime.

Sixthly, the spheroidal equation has led to many hundreds of pages of tabulations [84] and further numerical work e.g. in [82, 94], though the most recent of this states that this study is still open in some aspects.

Seventhly, one can furthermore envisage extending analogy A.2) to have the further parallel with our model that a rotationally-dislocated molecule in a cubic crystal will have preferred directions in space of approximately the same form as ours are in configuration space. We do not know if such a study has been done.

Finally, we comment that A.3) has been extended [95] to include what for us are C , D , E and F terms. For, what one has more generally is a symmetric polarization tensor α such that $\mu_\rho = \alpha_{\rho\sigma} \mathbf{E}_\sigma$. Then for the CO_2 model in a diagonal basis $\alpha_z = \alpha_{||}$ giving the combination $-\alpha_\perp \sin^2\theta - \alpha_{||} \cos^2\theta$ [a slight improvement of analogy A.3) by inclusion of the smaller $\alpha_\perp = \alpha_x = \alpha_y$], and this readily rearranges to the special case of the third form of (35). But for more general groups than just oxygen atoms at each end of the axis (while still remaining in a diagonal basis) $\alpha_x \neq \alpha_y$, giving $-\alpha_x \sin^2\theta \cos^2\phi - \alpha_y \sin^2\theta \sin^2\phi - \alpha_z \cos^2\theta$ which is the general case of the second form of (35). Moreover, in non-diagonal bases, the off-diagonal elements form extra terms directly analogous to those in (37). Thus there is an extended analogy between our problem and the study of polarization, with 4-stop metroland’s Jacobi–Hooke coefficients forming a configuration space-indexed analogue of the spatial-indexed polarizability tensor.

4 Conclusion

Relational particle models (RPM’s) benefit from notions of locality and structure that are absent in minisuperspace and are free of many of the technical difficulties of midisuperspace models. This makes them suitable for testing some of the conceptual aspects of quantum cosmology, and of quantum general relativity (such as the Problem of Time). In particular, in this paper we study the RPM of 4 particles in 1- d – 4-stop metroland – in the case without scale, both classically and quantum-mechanically. We concentrate on the clustering into two particular binary clusters [of particles {12} and particles {34}] both by using coordinates that follow this case and imposing a potential term that restricts the physics to being near such a configuration. This is toward a qualitative conceptual model of the quantum cosmological seeding of structure formation in a semiclassical regime (paralleling the Halliwell–Hawking [52] approach, which is somewhat narrower as a Problem of Time strategy but has further conceptual and computational applications outside of the Problem of Time context too), and of records theory [43, 55, 45, 4, 56, 57]. The counterpart of the current paper’s model with scale (which is harder and in which the current paper’s work occurs as a subworking under the shape–scale split) will be required for some aspects of such a study (in particular, for a semiclassical treatment with a greater number of parallels to that of GR). This is further work in progress [10, 11, 12, 28], though Sec 4.2–4 give a brief account of generalizations of the current paper’s model and how these meet additional quantum cosmological and Problem of Time criteria.

This paper’s model has an S^2 configuration space and then the mathematics which follows has analogies with the standard axisymmetric sphere and central force problems of ordinary mechanics. In particular, where a conserved angular momentum occurs in these analogue problems, a conserved relative dilational momentum occurs in our model. [These both have $SO(3)$ mathematics, but each has a different physical nature, the two being embraced by our notion of rational momentum which generalizes angular momentum to ratios that do not happen to physically be angles.] We then interpret some of 4-stop metroland’s classical and quantum solutions in cases with harmonic oscillator-like potentials. The solutions in spherical variables give fairly standard mathematics such as that of the rigid rotor and of the 2- d isotropic harmonic oscillator in some of the simpler cases, albeit now these require subsequent interesting and unusual interpretation in terms of the 4-stop metroland problem’s mechanical variables. We deduce this at the level of mass-weighted coordinates by tessellating the shape space sphere by the mechanical interpretation appropriate to 4-stop metroland, which we find to possess the symmetry group of the cube. Further tools we introduce, paralleling basic treatises on the atom, are expectations and spreads of shape operators, to which we can also attribute cosmological analogies. Our shape operators are RelSize(12,34): the relative size difference between universe and its {12}, {34} cluster contents, RelSize(1,2): the size of the {12} cluster relative to the size of the whole model universe, and its {34} cluster counterpart. The polar angle Φ itself is an inhomogeneity ratio of the contents of the universe themselves (i.e. of the two clusters relative to each other).

We obtain expectations and spreads for such operators e.g. for the ground state and for large quantum number limits. We consider the very special constant potential case that resides within the harmonic oscillator-like potential models as a particularly structurally homogeneous balance of springs, as well as more general cases treated perturbatively for small differences in spring constitution, asymptotically for large such differences, and in near-polar approximations. We further benefit from recognizing that the special case with the two clusters of the same spring constitution but the inter-cluster spring is weaker gives an otherwise well-known spheroidal equation, alongside various molecular physics analogies: with H_2^+ , NH_3 , rotation of molecules in crystals and molecular polarizability (at least the last of which extends to cases with more general combinations of springs between the four particles). This permits us to tap into substantial mathematical physics results and generally control our particular problem, and is a further example of useful bridges between RPM quantum cosmology models and the physics of molecules (triangleland RPM with harmonic oscillator-like potentials having already been found to share mathematics with the Stark effect for a linear rigid rotor [19]).

4.1 Comments on extension to $N > 4$ metrolands

The Jacobi H- and K-coordinates of Fig 1 generalize to an increasing variety of ‘part H-shaped, part K-shaped’ clusterings ([96] may be useful in this respect), which are of additional value as less trivial models of structure formation and of records theory. For full reduction for scalefree arbitrary- N -stop metroland and the subsequent Euler–Lagrange equations in the arbitrary-potential case, see [18, 9]. Moreover, we now comment that the number and nature of conserved quantities that each of these possesses is tied to the usual $SO(N - 1)$ representation theory, and their physical interpretations extend the present paper’s discovery of dilational quantities. Tessellations by physical interpretation are now harder as they both have more pieces and also are more difficult to visualize due to being higher-dimensional. However, our relative size and contents inhomogeneity shape operators do straightforwardly extend to N -stop metroland.

Within each N -stop metroland, one can envisage a tower of special, very special, ... (very) $^{N-2}$ special problems. The most special of these in each case has a constant potential and thus gives ultraspherical geodesics classically and the ultraspherical rigid rotor quantum-mechanically (solved by ultraspherical harmonics [19]), while the next most special of these in each case has $(N - 1)$ - d isotropic harmonic oscillator mathematics in its near-polar regime (solved by a power times a Gaussian times an associated Laguerre polynomial). Establishing a perturbative regime about each most special problem would then appear to be possible e.g. [19] by recurrence relations of the Gegenbauer polynomials [82, 98]. One technical difference is that, if one does use conformal operator ordering, then one can no longer use the configuration space being $2-d$ to evoke collapse to Laplacian ordering like in Sec 3.1. However, hyperspheres are of constant curvature and so of constant Ricci scalar curvature, so $\xi \text{Ric}(\mathbb{S}^k)$ is just a constant, $\xi k\{k - 1\}$ (our ‘E has no nonconstant prefactors banal conformal representation’ having the unit sphere as its configuration space). So, even in this case, the sole difference between Laplace and conformal ordering [or any other member of the $D^2 - \xi \text{Ric}(M)$ family of operators] is in what is to be interpreted to be the zero of the energy. We also note that for $N = 5$ the analogy with the Halliwell–Hawking scheme is somewhat tighter, as both involve perturbative expansions in \mathbb{S}^3 ultraspherical harmonics. Finally, the next most special equation unapproximated can also be mapped to the spheroidal equation, so that the fairly standard mathematical physics of that equation continues to be of aid in N -stop metroland.

4.2 Comments on Extension to metrolands with scale

The configuration spaces for these are cones over the corresponding shape spaces [11]. The present paper’s advances in the physical understanding of conserved quantities in RPM’s have further applications here. Our introduction of shape quantities to be promoted to operators also continues to be relevant here through there being a shape–scale split, so that evaluating shape operators here collapses back to pure shape workings such as the present paper’s. Expectation and spread of size (in close parallel with atomic physics) will also now be pertinent. Metrolands with scale will now have solid rather than surface analogues of the present paper’s ‘tessellation by physical interpretation’ technique. The way in which similarity RPM arises as a subproblem from the shape-scale split of the scaled theory means that the most special harmonic oscillator case and perturbations thereabout survives as a piece of the analysis upon introduction of scale, now partnered by isotropic harmonic oscillators in the size quantity.

This setting with scale is more appropriate as regards toy-modelling of cosmology in general and using a semiclassical approach in particular, both in the Problem of Time context and as a toy model of the Halliwell–Hawking approach [52]. One of us provides a first sketch at this in the smallest case in [10], with other cases to follow in [11, 12, 28], involving more realistic early universe cosmology dynamics of scale with the RPM (square root of) the moment of inertia I playing the role of the GR scalefactor a , coupled now to light, fast RPM shape dynamics that is easier to solve than GR’s corresponding quantum dynamics of inhomogeneities. We also note that, even in 1-d with scale (for which there are no linear constraints), RPM’s still have the important nontriviality of possessing a notion of localization/inhomogeneity/structure (while minisuperspace has neither this nor linear constraints). Finally, inclusion of scale is also *necessary* if one’s RPM is to have a hidden time [17, 8, 97] that parallels GR’s York time.

4.3 Comments on extension to $2-d$

The price to pay in introducing scale is that one no longer has nontrivial constraints in spatially $1-d$ models with which to model some effects due to GR’s momentum constraint. On the long term, one can get around this by passing to spatial dimension > 1 . A first such model is triangleland: the RPM of 3 particles in the plane. This has a \mathbb{S}^2 shape space like the present paper’s 4-stop metroland model does. This gives a number of useful insights. E.g. parts of the present paper parallel [9, 19]. Even more significantly, because the 4-stop metroland interpretation of the sphere turns out to be more straightforward, the present paper is useful as regards obtaining an improved understanding of the less straightforward triangleland case [20]. Scaled triangleland is harder; so far we have just provided some classical study for this (also to be augmented by the present paper’s techniques at the classical level in [11] toward finally providing a quantum study of it in [14]).

Moreover, triangleland lacks the present paper’s nice feature of splitting into two nontrivial subsystems (of 2 particles each), which is a useful nontriviality from the structure formation and records theory perspectives. Studying scaled quadrilateralland (RPM of 4 particles in the plane) [99] would incorporate this feature too. Thus this model would possess a number of midisuperspace’s features with the benefit of being technically simpler. This makes it particularly

suitable for the simultaneous investigation of records theory and the semiclassical approach (which may support each other, and histories theory, to form a more robust combined approach to the Problem of Time and to quantum cosmology [100, 56, 19]). Quadrilateralland does have a further technical complexity – its shape space is $\mathbb{C}\mathbb{P}^2$, which unavoidably involves complex-projective mathematics (triangleland has $\mathbb{C}\mathbb{P}^1$ but this is well-known to also be \mathbb{S}^2).

Further features for consideration in RPM models involve [13] A) oriented shapes – real projective spaces $\mathbb{R}\mathbb{P}^{N-2}$ in place of \mathbb{S}^{N-2} as shape spaces or $\mathbb{C}\mathbb{P}^{N-2}/\mathbb{Z}_2$ in place of $\mathbb{C}\mathbb{P}^{N-2}$ as shape spaces and the corresponding cones in models with scale and/or B) (partial) particle indistinguishability by which only pieces of whichever of the preceding spaces would pass to being the configuration spaces. The present paper’s treatment of physical interpretation by multiple coordinate charts and tessellations by physical interpretation are doubtlessly ideas of further value in the study of these models with their wide range of configuration space geometries.

4.4 Further details of Problem of Time and quantum cosmology applications

Our wavefunctions, eigenvalues and operators are useful in the following Problem of Time investigations.

1) The computation of naïve Schrödinger interpretation [53] probabilities of the universe having some particular property. Example 1) consider quantifying P(universe is large), in the sense that the two clusters under study are but specks in the firmament, by P(ϵ -close to the {12,34} double-double collision), which means, at the level of the configurations themselves, that the magnitude of $\sqrt{\text{RelSize}(1,2)^2 + \text{RelSize}(3,4)^2}/\text{RelSize}(12,34)$ lies between 1 and $1 - \epsilon^2/2$, and, in configuration space terms, that one is in the ϵ -caps about each pole. Then from the latter and by the naïve Schrödinger interpretation, this probability $\propto \int_{\epsilon\text{-caps}} |\Psi|^2 dS = \int_{\Phi=0}^{2\pi} \{ \int_{\Theta=0}^{\epsilon} + \int_{\Theta=\pi-\epsilon}^{\pi} \} |\Psi(\Theta, \Phi)|^2 \sin \Theta d\Theta d\Phi$. So, e.g. for the very special solution’s ground state and first excited state, one gets proportionality to $\epsilon^2 + O(\epsilon^4)$, while for the states with dilational quantum numbers $D = 1$, $|d| = 1$, one gets proportionality to $\epsilon^4 + O(\epsilon^6)$.

Example 2) consider quantifying P(the two clusters nominally under study are in fact merged) by P(δ -close to {12,34} merger) which means, at the level of the configurations themselves, that the size of $\text{RelSize}(12,34)$ does not exceed the small number δ , and, in configuration space terms, that one is in the δ -belt around the equator. Thus P(δ -close to {12,34} merger) $\propto \int_{\delta\text{-belt}} |\Psi|^2 dS$, which, in the very special case, works out to be proportional to $\delta^3 + O(\delta^5)$ for $D = 1$ $d = 0$ and to $\delta + O(\delta)^3$ for the other three lowest-lying states.

Example 3) consider quantifying P(universe is contents-homogeneous) in the sense that the two clusters under study are similar to each other, by the magnitude of $\text{RelSize}(1,2)/\text{RelSize}(3,4)$ departing from 1 by no more than 2η . Then, on configuration space, one is in the tetralune described in Fig 2, and the naïve Schrödinger interpretation gives P(universe is η -contents-homogeneous) $\propto \int_{\eta\text{-tetralune}} |\Psi|^2 dS$, which, in the very special case, comes out as proportional to η for all four of the lowest-lying states.

Example 1 also makes sense for the small-regime special solution. One now obtains proportionality to $\epsilon^2 \sqrt{\omega/\hbar}$ to leading order i.e. the same ‘(small)²’ factor as in the very special problem but now with an opposing ‘ $\sqrt{\text{large}}$ ’ factor, amounting to the small regime’s potential well (Fig 3b) concentrating the wavefunction near the poles i.e. in the region of the configuration space corresponding to large universes in the above-described sense.

Finally, also repeating Example 1 for the wavefunctions with first order perturbative corrections in B included, we now find proportionality to $\epsilon^2 \{1 - 8BI^2/9\hbar^2\} + O(B^2) + O(\epsilon^4)$ for the ground state, to $\epsilon^2 \{1 - 8BI^2/25\hbar^2\} + O(B^2) + O(\epsilon^4)$ for $D = 1$, $d = 0$, and $\epsilon^4 \{1 - 36I^2B/25\hbar^2\} + O(B^2) + O(\epsilon^6)$ for the $D = 1$, $d = 1$ states. The signs of these corrections conform with intuition, as (Fig 3a) $B > 0$ corresponds to placing a potential barrier at the poles and a well around the equator, which should indeed decrease the amount of wavefunction there, i.e. making large universes less probable, and vice versa for $B < 0$.

2) Given explicit wavefunctions such as this paper’s, one can build up projectors and mixed states (including with environment portions traced out) and then construct conditional probabilities [43] for pairs of universe properties.

3) As regards records theory [57], the current paper’s classical work provides some means of defining a notion of distance on configuration space (which is quite closely related to the measure problem in cosmology [54]), and a notion of localizability in space. Next [101], one would construct notions of information (alias negentropy) both at the classical level and at the quantum level for the problems solved in this paper. In this respect it is worth noting that QM perturbation theory suffices in order to build an approximate statistical mechanics [102]. Such notions of information include e.g. Shannon’s, von Neumann’s, Tsallis’s [57], as well as notions of subsystem information, mutual information and correlation (such as the covariance for the two clusters in the situation that the present paper centres on).

4) One can also build up decoherence functionals for histories theory [58], and consider the Feynman–Vernon influence functional that Halliwell uses [56] for the study of records within histories theory.

5) Exact wavefunctions also serve as useful checks on whether the semiclassical approach’s assumptions and approximations are appropriate [12, 28]. By the arguments in SSec 4.2, we prefer to wait until we have set up scaled models before carrying out such a study.

Some further quantum cosmological applications are as follows.

A) RPM’s are well-suited for the investigation of the issue of whether quantum cosmology is robust to neglecting some degrees of freedom. This was investigated by Kuchař and Ryan [103] for minisuperspace, though tractable minisuperspace examples of this are expected to be rare, while considering an $N - 1$ particle RPM within an N -particle RPM is more straightforward. There is however here the catch that, by relationally meaningful degrees of freedom counting, 4-stop

metroland is the smallest nontrivial SRPM, so one would need to study scalefree 4-stop metroland within as-yet not explicitly studied scalefree 5-stop metroland (or *scaled* 3-stop metroland within scaled 4-stop metroland).

B) RPM's are also useful toy models for whether uniform states have an important or privileged status [104]. E.g. examples 2 and 3 above can be interpreted as concerning aspects of uniformity, as can the parallel investigation of the probability of being close to the equilateral triangle configuration in [20].

We comment that [11] contains some further details of the above as toy models of aspects of GR alongside listing yet further applications.

We note that operator insertions for meaningful shape operators remain useful in constructing various of the above Problem of Time-relevant objects and schemes. All of 2) to 5) above have workings substantially longer than 1), or, alongside A), are better considered for extensions of the present paper's model (though this still features within as a submodel). Thus we leave further detail of these for future occasions. Finally, we comment that RPM's are mostly intended as qualitative models of conceptually-interesting features of quantum cosmology [though they are capable of testing the extent to which quantitative and observationally-tieable calculations in inhomogeneous GR quantum cosmology should be trusted, 5) and A) being clear examples of this, as well as permitting more comparison and composition of Problem of Time strategies than is usually possible, due to their high level of mathematical tractability].

4.5 Analogues of our shape operators in mini and midisuperspace?

Another longer-term goal would be to export insights acquired by our program to 'mini- and midi-'superspace; are there then useful analogues of shape operators for these (anisotropy operators, inhomogeneity operators?) In surveying the literature, we have found, firstly, that the abovementioned Kuchař and Ryan paper considers $\langle y^2 \rangle$ for y a reparametrization of one of the anisotropy degrees of freedom β_{\pm} in diagonal Bianchi IX quantum cosmology. Secondly, Ashtekar and Bojowald make mention of an anisotropy operator in studying loop quantum gravity [105]. Thirdly, Petryk and Schleich [106] consider expectation values for geometrical quantities in the Hartle–Hawking initial state in their study of conditional probabilities in the 3- d Ponzano-Regge minisuperspace. Fourthly, Halliwell and Hawking [52] compute the expectation of the anisotropy in temperature of the microwave background; this has the additional value of being “halfway to midisuperspace” in that it considers inhomogeneous perturbations about a homogeneous spacetime. As regards inhomogeneous spacetimes, the Lemaître–Tolman–Bondi solution principally concerns radial scale variables, so it is far more of an analogue to the shape-scale extension of the present paper. While there is not anything as yet that we know about using shape operators at the quantum level for the Gowdy universe, e.g. Andersson, van Elst and Uggla [107] use a form of shape-scale variables at the classical level. Thus, while shape quantities and shape operators have occasionally been used in 'mini and midi'superspace, a systematic treatment paralleling that in atomic physics does as yet appear to be lacking.

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Appendix A This paper's generalization of angular momentum put into context

What is habitually called angular momentum mathematics (because that is a common guise in which it appears in physics), is, structurally, the representation theory of $SO(p)$. The most usual case is that of $SO(3)$, habitually called the rotation group, and also interpretable as the isometry group of the 2-sphere [more generally, $SO(p)$ is the p -dimensional rotation group and the isometry group of the $(p - 1)$ -sphere]. In turn, $SO(3)$ is closely related to $SU(2)$ (which is its double cover). The rational momentum viewpoint is more general than the mechanical angular momentum perspective but not the $SO(p)$ one, as Fig 6 begins to explain by classifying examples. Beyond that, $SO(p)$ can arise as a piece of an even larger group. [This is already the case for Fig 6's Runge–Lenz example, which can be viewed as a second $SO(3)$ coming from a partly-'hidden' $SO(4)$, but it covers further cases where the group is not necessarily 'hidden', such as $SO(3, 1)$ in relativistic particle physics, or $SU(3)$ containing 3 different directions' worth of $SU(2)$ ladder operators]. Quantum 'SO(p) objects' also combine under an addition rule, whereby composites of cases in Fig 6 arise. E.g. total angular momentum $T = L + S$ in atomic physics; more generally, total rational momentum $\mathcal{T} = \mathcal{R} + \mathcal{A}$, which also would include the effect of adding internal 'arrows' to the present paper's 1- d RPM setting.⁹ There are also rational momenta that are linear combinations of relative angular momentum and relative dilational momenta occur in triangle-land [20]. In this sense, this paper's rational momentum came about from building a different notion of 1- d space from the usual into the present paper (scalefreeness) Finally, adding arrows to the present model could be nontrivial in the sense that the 1- d arrows need not just obey separate 'tensored-on' occupation rules since dilational momentum exists as does addition of arrow and dilational momentum quantities, so that spatially 1- d models can have arrow-dilational momentum interactions that parallel the spin-orbital angular momentum couplings that occur in higher spatial dimensions.

⁹As the word 'spin' itself has rotational and hence angular momentum connotations, we generalize 'spin alias internal angular momentum', S , to 'arrow alias internal rational momentum', \mathcal{A} .

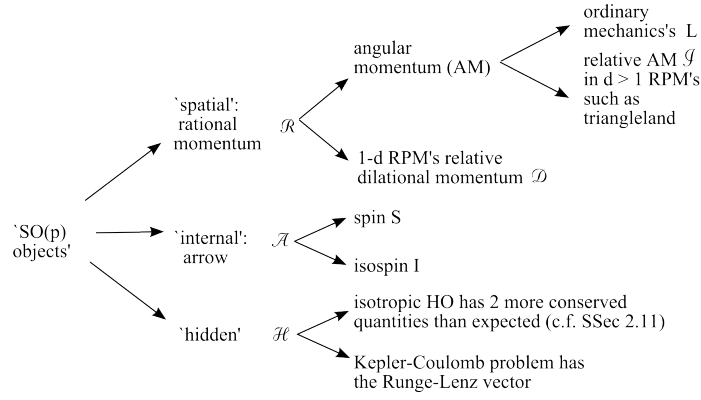


Figure 6: Various physical realizations of SO(p) objects.

Appendix B Some results concerning associated Laguerre Polynomials

The bounded solutions of the associated Laguerre equation

$$\xi y_{,\xi\xi} + \{\alpha + 1 - \xi\} y_{,\xi} + \beta y = 0 \quad (83)$$

are the associated Laguerre polynomials $L_{\beta}^{\alpha}(\xi)$. These obey [82] the orthogonality relation

$$\int_0^{\infty} \xi^{\alpha} \exp(-\xi) L_{\beta}^{\alpha}(\xi) L_{\beta'}^{\alpha}(\xi) d\xi = 0 \text{ unless } \beta = \beta' \quad (84)$$

and the recurrence relation

$$\xi L_{\beta}^{\alpha}(\xi) = \{2\beta + \alpha + 1\} L_{\beta}^{\alpha}(\xi) - \{\beta + 1\} L_{\beta+1}^{\alpha}(\xi) - \{\beta + \alpha\} L_{\beta-1}^{\alpha}(\xi) . \quad (85)$$

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