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Why Liquids? A Symmetry-Based Solution to Weisskopf's Challenge

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Abstract

In 1977, the renowned physicist Victor Weisskopf challenged the physics community to provide a fundamental explanation for the existence of the liquid phase of matter. A recent essay confirms that Weisskopf's 1977 question remains a challenge. In this paper, we use natural symmetry ideas to show that liquids are actually a natural state between solids and gases.

Keywords: liquids, symmetry groups, foundations of physics

1 Formulation of the Problem

Weisskopf's challenge: original formulation. In his 1977 essay [2], the renowned physicist Victor Weisskopf challenged the physics community to provide a fundamental explanation for the existence of liquids. Solid bodies, in their crystal form, with their natural symmetries, correspond to the state with the smallest possible energy – the state that most materials take at the absolute zero temperature (O° Kelvin, which is approximately $-273°$ C). Gases, with no restriction on their shapes, are also a natural state – they correspond to high temperatures. When heated, solid bodies eventually become gases – usually, with an intermediate liquid state. But how to explain this intermediate state?

Weisskopf's challenge: current status. A recent essay [1], while overviewing the progress in answering this question, confirms that Weisskopf's 1977 question remains a challenge.

What we do in this paper. In this paper, we use natural symmetry ideas to show that liquids are actually a natural state between solids and gases.

2 Towards a Formulation of the Problem in Precise Terms

Local transformations. In nature, most processes are smooth, so it makes sense to consider only smooth (differentiable) transformations.

All states allow shifts, so we will look for transformations beyond shifts.

Locally, in the vicinity of each point $(x_1^{(0)}, \cdots, x_n^{(0)})$, i.e., for points

$$(x_1, \cdots, x_n) = (x_1^{(0)} + \Delta x_1, \cdots, x_n^{(0)} + \Delta x_n),$$

we can expand each smooth transformation

$$(x_1, \cdots, x_n) \to (y_1, \cdots, y_n) = (f_1(x_1, \cdots, x_n), \cdots, f_n(x_1, \cdots, x_n))$$

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in Taylor series and keep only linear terms in this expansion. Then:

$$y_i = f_i(x_1, \cdots, x_n) = f_i(x_1^{(0)} + \Delta x_1, \cdots, x_n^{(0)} + \Delta x_n) \approx y_i^{(0)} + \sum_{j=1}^{n} a_{ij} \cdot \Delta x_j,$$

where

$$y_i^{(0)} \stackrel{\text{def}}{=} f_i(x_1^{(0)}, \cdots, x_n^{(0)})$$

and

$$a_{ij} \stackrel{\text{def}}{=} \frac{\partial f_i}{\partial x_j}_{|(x_1^{(0)}, \cdots, x_n^{(0)})}.$$

Since shift is always possible, we can apply the shift by $x_i^{(0)} - y_i^{(0)}$, thus getting a new transformation

$$(x_1^{(0)} + \Delta x_1, \cdots, x_n^{(0)} + \Delta x_n) \to (y_1, \cdots, y_n) = \left(x_1^{(0)} + \sum_{j=1}^{n} a_{1j} \cdot \Delta x_j, \cdots, x_n^{(0)} + \sum_{j=1}^{n} a_{nj} \cdot \Delta x_j \right).$$

In terms of the differences $\Delta y_i \stackrel{\text{def}}{=} y_i - x_i^{(0)}$, this local transformation becomes linear homogeneous:

$$\Delta y_i = \sum_{j=1}^{n} a_{ij} \cdot \Delta x_j.$$

So, locally, it is sufficient to consider linear transformations.

Local Lie group: a brief reminder. Clearly, if two transformations are possible, then their composition is also possible. Also, if a transformation is possible, then an inverse transformation is also possible. In mathematics, classes of transformations which are closed under composition and under taking the inverse are known as *groups*. In these terms, transformations form a group.

The set of all possible transformations usually smoothly depends on some parameters. In mathematics, such transformation groups are called *Lie groups*. Local transformations form a *local Lie group*.

Local (linear) transformations are uniquely determined by the corresponding matrices a_{ij}. One can easily see that the composition of two transformations corresponds to the product of the two matrices, and the inverse transformation corresponds to an inverse matrix. Thus, the local Lie group is a class of matrices which is closed under matrix multiplication and taking the inverse.

Lie algebras: a brief reminder. Each transformation occurs during a certain time period T, during which the original state smoothly turns into the new state. At each moment of time $t \le T$, we have some intermediate stage of this transformation. We can thus divide the interval of width T into several small subintervals of size $\Delta t \ll T$, and consider the whole transformation as a composition of transformations from moment 0 to moment Δt, from moment Δt to moment $2\Delta t$, etc., until we reach moment T. Let us denote the transformation from moment t to moment t' by $a_{ij}(t, t')$. In these terms, the transformation from a moment t to the next moment $t + \Delta t$ has the form $a_{ij}(t, t + \Delta t)$. For $t' = t$, the transformation is the identity matrix $a_{ij}(t, t) = \delta_{ij}$, where $\delta_{ii} = 1$ for all i and $\delta_{ij} = 0$ for all $i \neq j$.

Since the transformation is smooth, we can expand the dependence $a_{ij}(t, t + \Delta t)$ in Taylor series and keep only terms linear in Δt in this expansion:

$$a_{ij}(t, t + \Delta t) \approx a_{ij}(t, t) + b_{ij}(t) \cdot \Delta t = \delta_{ij} + b_{ij}(t) \cdot \Delta t, \tag{1}$$

where

$$b_{ij}(t) \stackrel{\text{def}}{=} \frac{\partial a_{ij}(t, t')}{\partial t'}_{|t'=t}.$$

In mathematical terms, the above transformation (1) – corresponding to very small time intervals Δt – is called *infinitesimal*, and the class of all such transformations is known as a *Lie algebra*.

Each transformation can be represented as a composition of transformations corresponds to small time intervals Δt. Once we know the corresponding Lie algebra, we can describe each such transformation with good accuracy and thus, describe the original transformation as their composition. The smaller Δt, the more accurate this representation. This means that, once we know the Lie algebra, we can determine all possible transformations with any desired accuracy.

So, to describe the class of all possible transformations, it is sufficient to describe the corresponding Lie algebra.

Natural properties of Lie algebras: reminder. If we have two infinitesimal transformations, with matrices $a'_{ij} = \delta_{ij} + b'_{ij} \cdot \Delta t$ and $a''_{ij} = \delta_{ij} + b''_{ij} \cdot \Delta t$, then the matrix a_{ij} describing their composition is equal to the product of these matrices:

$$a_{ik} = \sum_{j=1}^{n} a'_{ij} \cdot a''_{jk} = \sum_{j=1}^{n} (\delta_{ij} + b'_{ij} \cdot \Delta t) \cdot (\delta_{jk} + b''_{jk} \cdot \Delta t).$$

Opening parentheses and ignoring terms proportional to $(\Delta t)^2$, we conclude that

$$a_{ik} = \sum_{j=1}^{n} \delta_{ij} \cdot \delta_{jk} + \sum_{i=1}^{n} \delta_{ij} \cdot b''_{jk} \cdot \Delta t + \sum_{j=1}^{n} b'_{ij} \cdot \delta_{jk} \cdot \Delta t.$$

Taking into account that only the diagonal values of the unit matrix δ_{ij} are non-zeros – and that these diagonal elements are equal to 1 – we conclude that

$$a_{ik} = \delta_{ik} + (b'_{ik} + b''_{ik}) \cdot \Delta t.$$

Thus, the composition of two transformations corresponds to the sum of the matrices from Lie algebra. So, the Lie algebra should be closed under addition.

Similarly, one can show that the inverse corresponds to $-b_{ij}$, and that, in general, for each real number λ and for each matrix b_{ij}, the Lie algebra also contains the matrix $\lambda \cdot b_{ij}$. Combining this property with addition, we can conclude that each Lie algebra contains an arbitrary linear combination of its elements.

Resulting formulation of the problem. For a solid body, the only possible transformations are shifts and rotations. Thus, the only possible local transformations are rotations. It is known that the corresponding Lie algebra A_s (s for *s*olid) consists of all antisymmetric matrices b_{ij}, i.e., matrices for which $b_{ji} = -b_{ij}$ for all i and j.

For the gas, all smooth transformations are possible. Thus, the corresponding Lie algebra L_g (g for *g*as) consists of all the matrices b_{ij}.

In these terms, the question is: what are the Lie algebras L which are strictly larger than L_s but strictly smaller than L_g, i.e., algebras for which $L_s \subset L \subset L_g$?

3 Main Result

Proposition. *There are exactly two Lie algebras L that strictly contain the algebra L_s of all antisymmetric matrices and that are strictly contained in the algebra L_g of all matrices:*

- *the algebra L_l that consists of all matrices with zero trace* $\mathrm{Tr}(b) \stackrel{\text{def}}{=} \sum_{i=1}^{3} b_{ii} = 0$, *and*
- *the algebra L_a obtained by adding all scalar matrices $\lambda \cdot \delta_{ij}$ to antisymmetric ones.*

Discussion. Liquids are (largely) incompressible – this is their main difference from gases. This means that they are characterized by transformations that preserve volume. In terms of Lie algebras, preserving volume means exactly $\mathrm{Tr}(b) = 0$. Thus, our result indeed explains the existence of liquids.

We also have another case. These additional elements of Lie algebra correspond to increasing and decreasing the size of the object without changing its proportions. This may correspond to some yet unknown state of nature.

Proof.

1°. Let L be a Lie algebra that strictly contains L_s and that is strictly contained in L_g. Let us first show that the algebra L contains a matrix b_{ij} if and only if it contains its symmetric part $b^{\text{sym}}_{ij} \stackrel{\text{def}}{=} (b_{ij} + b_{ji})/2$.

Indeed, each matrix b_{ij} can be represented as a sum of its symmetric part and an antisymmetric part $b_{ij}^{\rm asym} \stackrel{\rm def}{=} (b_{ij} - b_{ji})/2$. Since the class L is closed under addition and contains the class L_g of all antisymmetric matrices, this means that if the symmetric part of b_{ij} is in L, then the original matrix b_{ij} is also in L, as the sum of two matrices $b_{ij}^{\rm sym}$ and $b_{ij}^{\rm asym}$ from the class L.

Vice versa, since the class L is closed under linear combination, for each matrix b_{ij}, the class L contains the matrix $b_{ij} - b_{ij}^{\rm asym}$, which is exactly the symmetric part of the matrix b_{ij}.

2°. Due to Part 1 of the proof, to describe all the matrices from the class L, it is sufficient to describe all symmetric matrices from this class.

3°. Since the Lie algebra contains all antisymmetric matrices, the corresponding transformation group contains all rotations T. One can easily check that if we first apply the rotation T, then an infinitesimal transformation with matrix $B = \|b_{ij}\|$, and then inverse rotation T^{-1}, we get an infinitesimal transformation with matrix $T^{-1}BT$. Thus, with each matrix B, the Lie algebra L contains all the matrices obtained from it by a rotation.

It is known that each symmetric matrix, by an appropriate rotation – in which coordinates axes are rotated into the matrix's eigenvectors – can be transformed into a diagonal form. Thus, to describe all symmetric matrices from L, it is sufficient to describe all diagonal matrices from the class L.

4°. Let us prove that if L contains at least one matrix with $\mathrm{Tr}(b) \neq 0$, then it contains all scalar matrices.

Indeed, if the algebra A contains one matrix with non-zero trace, then its diagonal form $b = \mathrm{diag}(b_{11}, b_{22}, b_{33})$ will have the same trace $\mathrm{Tr}(b) = b_{11} + b_{22} + b_{33} \neq 0$. Thus, due to rotation-invariance, it also contains matrices $\mathrm{diag}(b_{22}, b_{33}, b_{11})$ and $\mathrm{diag}(b_{33}, b_{11}, b_{22})$ obtained from the original one by a rotation that changes the coordinate axes. Hence, it contains the sum of these three matrices – which is a scalar matrix $\mathrm{Tr}(b) \cdot \delta_{ij}$. Every other scalar matrix can be obtained from this one by multiplying by a number; thus, every scalar matrix indeed belongs to L.

5°. Let us now prove that if L contains at least one non-scalar symmetric matrix, then it contains all matrices with $\mathrm{Tr}(b) = 0$.

Indeed, let us assume that L contains a non-scalar symmetric matrix. Then, its diagonal form $b = \mathrm{diag}(b_{11}, b_{22}, b_{33})$ is also non-scalar and symmetric. If $\mathrm{Tr}(b) \neq 0$, then, by Part 4 of this proof, all scalar matrices are also in L, in particular, a scalar matrix $(\mathrm{Tr}(b)/3) \cdot \delta_{ij}$ with the same trace. Subtracting this scalar matrix from b, we get a new non-scalar symmetric matrix from the algebra L whose trace is 0. Thus, without losing generality, we can assume that the original non-scalar symmetric matrix has trace 0. Since the matrix is non-scalar, at least two diagonal values b_{ii} are different from each other. Without losing generality, we can assume that $b_{11} \neq b_{22}$.

If we rotate by 90 degrees in the x_1-x_2-plane, we get a new diagonal matrix $b'_{ij} = \mathrm{diag}(b_{22}, b_{11}, b_{33})$. Subtracting b'_{ij} from b_{ij}, we get yet another diagonal matrix from the algebra L: the matrix

$$\mathrm{diag}(b_{11} - b_{22}, b_{22} - b_{11}, 0).$$

Since the Lie algebra is closed under multiplication by a scalar, we thus conclude that the diagonal matrix $\mathrm{diag}(1, -1, 0)$ also belongs to L.

By rotation, we can conclude that $\mathrm{diag}(0, 1, -1) \in L$. Now, each diagonal matrix with 0 trace has the form $\mathrm{diag}(p, q, -(p+q))$. We can represent this matrix as a linear combination of matrices from L:

$$\mathrm{diag}(p, q, -(p+q)) = p \cdot \mathrm{diag}(1, -1, 0) + (p+q) \cdot \mathrm{diag}(0, 1, -1).$$

Thus, every diagonal matrix with 0 trace belongs to L, and hence, every symmetric matric with 0 trace belongs to L.

6°. Now, we are ready to prove the proposition. Since $L_s \subset L$ and $L \neq L_s$, we conclude that L must contain at least one matrix which is not antisymmetric, and thus, must contain at least one symmetric matrix – namely, the result of its symmetrization.

If L contains a non-scalar matrix and a matrix with non-zero trace, then L contains all scalar matrices and all symmetric matrices with zero trace. Each symmetric matrix can be represented as a sum of the corresponding scalar part and zero-trace part, so this would mean that L contains all symmetric matrices – and thus, all of them. This contradicts to our assumption that $L \neq L_g$. So, L cannot contain both types of matrices.

Thus, we have two options:

- The first option is that L contains a non-scalar matrix. In this case, according to Part 5 of the proof, L contains all matrices with 0 trace, and, as we have just proved, it cannot contain any matrix with non-zero trace. In this case, L is the set of all matrices with 0 trace, i.e., $L = L_l$.

- The second option is that L contains a symmetric matrix with non-zero trace. In this case, L contains all scalar matrices – and, as we have just shown, it cannot contain any non-scalar symmetric matrix. This is the second case $L = L_a$.

The proposition is proven.

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