ICOSAHEDRAL SYMMETRY OF A POLYTOPE MODEL OF GLASS

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ABSTRACT

Short range order in metallic glasses is related to an ordered "crystal" of 120 atoms in S^3 known as "Polytope {3,3,5}". In this paper we exploit the rotational symmetries of the polytope to study the eigenstates of a tight binding Hamiltonian. The calculation relies on the homomorphisms between SU(2) and SO(3) and between SU(2) $\times$ SU(2) and SO(4). In addition the isomorphism of S^3 and SU(2) allows us to express the geometry of Polytope {3,3,5} in terms of the algebra of Y', the symmetry group of an icosahedron.

1. Introduction

Consider the behavior of a liquid metal as it is cooled to $T=0$.[1] If the cooling is sufficiently slow then at a temperature T_f the liquid freezes to a face centered cubic crystalline solid and the density increases discontinuously. If the cooling is sufficiently rapid no crystal is formed and instead we find a metallic glass. The density of this metallic glass is below that of the face centered cubic crystal. If we perform the same experiment on a moderate number of atoms instead of the bulk liquid we find a cluster that is neither a glass nor a fragment of face centered cubic crystal. Termed "Amorphons",[2] these clusters are actually highly ordered and tend to display icosahedral coordination. The density of these amorphons is greater than that of the face centered cubic crystal. Metallic glass is believed to consist of regions of high density icosahedral order interrupted by defects which arise from the frustration[3] associated with the tiling of $\mathbb{R}^3$ with icosahedra.

This frustration is relieved by curving space so that the atoms sit in S^3 rather than $\mathbb{R}^3$. Coxeter[4,5] has shown that 120 atoms can be arranged in S^3 in such a way that each atom sits at the center of an icosahedron and it's twelve nearest neighbors sit at the vertices of the icosahedron. This structure is known as Polytope {3,3,5}. Related constructions have been used to describe amorphous semiconductors and other materials.[6] In the following section we show how Polytope {3,3,5} is related to Y', the lift into SU(2) of the rotational symmetry group Y of an icosahedron. It then follows that the symmetry group G of the polytope is simply related to Y'. We use this relationship in section 3 to project certain irreducible representations of G out of the hyperspherical harmonics. An earlier paper[7] describes the relevance of these projections to x-ray scattering and electronic structure of the polytope.

2. Polytope {3,3,5}

Reference 3 shows a projection of the 120 vertices and 720 near neighbor bonds of the polytope {3,3,5}. To efficiently deal with symmetries of this object we need a concise way to enumerate the vertices and bonds. An especially useful enumeration exploits the isomorphism[8,9] between points on the four dimensional sphere S^3 and the group SU(2). A point $\hat{u} \in S^3$ can be thought of as a unit four-vector with components

$$\hat{u} = (\cos\psi,\ n_x \sin\psi,\ n_y \sin\psi,\ n_z \sin\psi) \tag{1}$$

where $\hat{n} = (n_x, n_y, n_z) \in S^2$ is a unit three-vector. Alternatively we can write $\hat{u}$ as an SU(2) matrix u through the identification

$$\hat{u} \to u \equiv 1 \cos\psi + i\hat{n}\cdot\sigma \sin\psi \tag{2}$$

where 1 is the 2×2 unit matrix and the σ_i are Pauli matrices.

Two points $u, v \in S^3$ can now be multiplied together by using the multiplication rules of Pauli matrices. The sphere S^3 has now been given the algebraic structure of the group SU(2). Henceforth we shall regard points in S^3 as synonomous with SU(2) matrices. As demonstrated in the book by DuVal,[8] the vertices of {3,3,5} can be identified with the lift into SU(2) of the sixty element icosahedral point group Y. The one hundred twenty element group Y' which results is known as the double group of Y. Because of its importance we shall summerize the properties of Y' which will be used in this paper.

The two element lift of an SO(3) rotation $R_{\hat{n}}(\theta)$ into SU(2) is given by the pair of matrices $\pm e^{1/2\ i(\hat{n}\cdot\vec{\sigma})\theta}$. The symmetry group Y of an icosahedron contains five conjugacy classes. The group Y' which is the lift of Y into SU(2) contains nine conjugacy classes. The identify in Y lifts to the classes

$$\gamma_0 = 1 \tag{3a}$$

and

$$\gamma_1 = -1 \tag{3b}$$

The twelve rotations by $2\pi/5$ lift to the classes

$$\gamma_2 = \left\{ e^{1/2\ i(\hat{n}\cdot\vec{\sigma})2\pi/5} : \hat{n} \text{ points to vertices of icosahedron} \right\} \tag{4a}$$

and

$$\gamma_3 = \{-u : u \in \gamma_2\} \quad . \tag{4b}$$

The twelve rotations by $\pm 4\pi/5$ lift to the classes

$$\gamma_4 = \{u^2 : u \in \gamma_2\} \tag{5a}$$

and

$$\gamma_5 = \{-u^2 : u \in \gamma_2\} \quad . \tag{5b}$$

The twenty rotations by $\pm 2\pi/3$ lift to the classes

$$\gamma_6 = \left\{ e^{1/2\ i(\hat{n}\cdot\vec{\sigma})2\pi/3} : \hat{n} \text{ points to faces of icosahedron} \right\} \tag{6a}$$

and

$$\gamma_7 = \{-u : u \in \gamma_6\} \quad . \tag{6b}$$

Finally, the fifteen rotations by π lift to the class

$$\gamma_8 = \left\{ e^{1/2\ i(\hat{n}\cdot\vec{\sigma})\pi} : \hat{n} \text{ points to edges of icosahedron} \right\} \quad . \tag{7}$$

Note that the elements of Y' depend on the orientation of the icosahedron through the directions $\hat{n}$. We shall always take $\hat{z}$ to be a 5-fold axis and $\hat{y}$ to be a 2-fold axis. This defines a "standard" orientation of Y'.

To study the geometry of the polytope it is useful to consider the geodesic seperation between two arbitrary points $u, v \in S^3$. Because the sphere has unit radius the seperation is just the angle between u and v

$$\psi(u,v) = \cos^{-1}\left(\frac{1}{2}\mathrm{Tr}\,\{uv^+\}\right) \tag{8}$$

where $v^+ = v^{-1}$ is the Hermitian conjugate of v. Note that the nearest neighbor vertices of the "North Pole" $u = 1$ comprise the class $\gamma_2 \subset Y'$. Consequently the nearest neighbors of any vertex $u \in Y'$ can be written vu where $v \in \gamma_2$. This shows that Y' indeed corresponds to Polytope $\{3,3,5\}$ since each vertex $u \in Y'$ has twelve nearest neighbors vu arranged at the vertices of an icosahedron centered at u.

We can now employ some facts[8,9] about $SO(4)$ to determine the symmetry group $G \subset SO(4)$ of Polytope $\{3,3,5\}$. Consider two points $u, v \in S^3$ and multiply them on the left by $\ell \in S^3$

$$u \rightarrow \ell u \tag{9a}$$

$$v \rightarrow \ell v \tag{9b}$$

or the right by $r^+ = r^{-1}$, $r \in S^3$,

$$u \to ur^{-1} \tag{10a}$$

$$v \to vr^{-1} \quad . \tag{10b}$$

Because of the group structure of S^3 the results of these multiplications are new elements of S^3. It follows from equation (8) that the geodesic separation is unchanged.

$$\psi(\ell u, \ell v) = \psi(ur^{-1}, vr^{-1}) = \psi(u,v) \tag{11}$$

Thus, the transformations in equations (9) and (10), called left and right screws respectively, are rotations. Every rotation of S^3 is generated by a combination of left and right screws, and every pair $(\ell, r) \in SU(2) \times SU(2)$ generates a rotation[8,9] through

$$(\ell, r): u \to \ell u r^{-1} \quad . \tag{12}$$

Noting that (ℓ, r) and $(-\ell, -r)$ generate the same rotation, we have the formal result

$$SO(4) = [SU(2) \times SU(2)]/Z_2 \quad . \tag{13}$$

We can obtain a similar formula for G. For any elements $\ell, r \in Y'$ the left and right cosets $\ell Y'$ and $Y'r^{-1}$ give the original group Y' in a new orientation. Thus rotational symmetry group of Polytope $\{3,3,5\}$ is

$$G = (Y' \times Y')/Z_2 \tag{14}$$

and it's double group is

$$G' = Y' \times Y' \quad . \tag{15}$$

3. Representations and Wave Functions

In this section we consider irreducible representations of Y' and G'. Our motivation for this is a generalization of Bloch's theorem which tells us that the eigenfunctions of a Hamiltonian invariant under a symmetry group form the basis for irreducible representations of the group. We use this fact to diagonalize a simple tight binding Hamiltonian. A second application will be made in the calculation of "icosahedral harmonics" and their generalization to the polytope. The results presented here are a refinement of similar results published previously.[7]

The characters of a group H, which depend on the conjugacy class $\gamma \subset H$ and the representation ρ of H, will be denoted $\chi_\rho^H(\gamma)$. In particular

$$\chi_j^{SU(2)}(\ell) = \sin(2j+1)\psi_\ell / \sin \psi_\ell \tag{16}$$

is the character of $\ell = e^{i\psi_\ell \hat{n}\cdot\vec{\sigma}} \in SU(2)$ in the irreducible representation of SU(2) with the spherical harmonics Y_{jm} as a basis. Similarly[9)]

$$\chi_n^{SO(4)}(\ell,r) = \chi_{n/2}^{SU(2)}(\ell)\ \chi_{n/2}^{SU(2)}(r^{-1}) \tag{17}$$

is the character of $(\ell,r) \in SO(4)$ in the irreducible representation with the hyperspherical harmonics Y_{n,m_1m_2} as a basis.

The irreducible representations of Y' are contained in the spherical harmonics. Explicit basis functions for Y' were computed by McLellan[10)] and are listed in Table 1. In general

$$\rho_{\alpha,i} = \sum_m Q_{jm}^{\alpha i}\, Y_{jm} \tag{18}$$

is the ith element of the basis for ρ_α.

TABLE 1. Irreducible Representations of Y'.

representation	dimension	basis	character
ρ_0	1	Y_{00}	$\chi_0^{Y'} = 1$
ρ_1	3	Y_{1m}	$\chi_1^{Y'} = \chi_1^{SU(2)}$
ρ_2	3	$Y_{30}, \sqrt{\frac{3}{5}}\, Y_{3\pm2} \mp \sqrt{\frac{2}{5}}\, Y_{3\mp3}$	$\chi_2^{Y'} = \chi_3^{SU(2)} - \chi_3^{Y'}$
ρ_3	4	$Y_{3\pm1}, \sqrt{\frac{2}{5}}\, Y_{3\pm2} \pm \sqrt{\frac{3}{5}}\, Y_{3\mp3}$	$\chi_3^{Y'} = \chi_5^{Y'}\chi_6^{Y'}$
ρ_4	5	Y_{2m}	$\chi_4^{Y'} = \chi_2^{SU(2)}$
ρ_5	2	$Y_{1/2\ m}$	$\chi_5^{Y'} = \chi_{1/2}^{SU(2)}$
ρ_6	2	$\sqrt{\frac{7}{10}}\, Y_{\frac{7}{2}\pm\frac{3}{2}} \pm \sqrt{\frac{3}{10}}\, Y_{\frac{7}{2}\mp\frac{7}{2}}$	$\chi_6^{Y'} = \chi_{7/2}^{SU(2)} - \chi_{5/2}^{SU(2)}$
ρ_7	4	$Y_{3/2\ m}$	$\chi_7^{Y'} = \chi_{3/2}^{SU(2)}$
ρ_8	6	$Y_{5/2\ m}$	$\chi_8^{Y'} = \chi_{5/2}^{SU(2)}$

The simplicity of equation (15) allows us to express the character table of G' in terms of the character table of Y'. Conjugacy classes of G' have the form $\gamma_{mn} = (\gamma_m, \gamma_n)$ and irreducible representations of G', denoted $\rho_{\alpha\beta}$, transform like $\rho_\alpha\rho_\beta$. Thus the character table of G' is given[11)] by

$$\chi^{G'}_{\alpha\beta}(\gamma_{mn}) = \chi^{Y'}_{\alpha}(\gamma_m)\chi^{Y'}_{\beta}(\gamma_n) \quad . \tag{19}$$

In general we can write

$$\rho_{\alpha\beta,ij} = \sum_{m_1 m_2} Q^{\alpha\beta,ij}_{n,m_1 m_2} Y_{n,m_1 m_2} \quad . \tag{20}$$

The transformation properties of $\rho_{\alpha\beta}$ require that

$$Q^{\alpha\beta,ij}_{n,m_1 m_2} = Q^{\alpha i}_{n/2\ m_1} Q^{\beta j}_{n/2\ m_2} \quad . \tag{21}$$

Irreducible representations of G' have now been expressed in terms of hyperspherical harmonics.

Now that we have determined the irreducible representations of G' we can diagonalize a simple tight-binding Hamiltonian

$$H = \sum_{u \in Y'} \sum_{v \in \gamma_2} |u\rangle\langle vu| \quad . \tag{22}$$

It can be shown[7)] that only the "diagonal" representations of G' are eigenfunctions of H. Define

$$\psi_{\alpha,ij} = \sum_{u \in Y'} \rho_{\alpha\alpha,ij}(\omega)\,|\omega\rangle \tag{23}$$

and note that evaluation of $H\psi_\alpha$ requires evaluation of

$$S_\alpha(u) = \sum_{v \in \gamma_2} \rho_{\alpha\alpha,ij}(vu) \quad . \tag{24}$$

By the considerations of the proceeding paragraph we can write

$$\rho_{\alpha\alpha,ij}(vu) = \sum_{i'} M^{Y'}_{\alpha,i'i}(v)\ \rho_{\alpha\alpha,i'j}(u) \tag{25}$$

where $M^{Y'}_{\alpha}$ is the matrix representation of $v \in Y'$ in ρ_α. Thus

$$S_\alpha(u) = \sum_{i'} \left\{ \sum_{v \in \gamma_2} M^{Y'}_{\alpha,i'i}(v) \right\} \rho_{\alpha\alpha,i'j}(u) \quad . \tag{26}$$

The Matrix sum in brackets of equation (26) commutes with all elements of Y' and hence schurs lemma applies. Equation (26) simplifies to

$$S_\alpha(u) = \left\{ O(\gamma_2)\chi^{Y'}_{\alpha}(\gamma_2)/d_\alpha \right\} \rho_{\alpha\alpha,ij}(u) \tag{27}$$

where d_α is the dimension of representation ρ_α. Thus

$$H\psi_\alpha = -\sum_{u\in Y'} S_\alpha(u)\,|u> \tag{28}$$

$$= \frac{-O(\gamma_2)\chi_\alpha^{Y'}(\gamma_2)}{d_\alpha}\psi_\alpha \tag{29}$$

So we see that ψ_α is indeed an eigenfunction of H with eigenvalue

$$E = \frac{-O(\gamma_2)\chi_\alpha^{Y'}(\gamma_2)}{d_\alpha} \tag{30}$$

and degeneracy d_α^2. This agrees with the numerical data of Warner.[12)]

As a final application we prove a conjecture[7)] concerning the construction of the unit representation from a basis of hyperspherical harmonics. It is well known[13)] that

$$\rho_{0,0} = -\sqrt{\frac{7}{10}}\,Y_{6,-5} + Y_{6,0} + \sqrt{\frac{7}{11}}\,Y_{6,5} \quad . \tag{31}$$

is the unit representation of an icosahedron in the "standard" orientation. Equation (21) allows us to express the unit representation of Polytope {3,3,5} in the "standard" orientation as

$$\rho_{00,00} = \sum_{m_1 m_2} Q_{6m_1}^{00}\,Q_{6m_2}^{00}\,Y_{12,m_1 m_2} \tag{32}$$

where the Q_{6m}^{00} can be read off equation (32). This proves the factorization[7)] of $Q_{12,m_1 m_2}^{00,00}$.

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