Quantum mechanics II, Solutions 10 : Variational Principle and Mathematical Introduction to Groups & Representations

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Variational Principle

Problem 1 : Potential well

Summary The aim of this exercise is to understand the principle of the variational method. We consider the problem of an infinite 1D potential well, defined by :

$$V(x) = \begin{cases} 0 & \text{if} \quad |x| < a \\ +\infty & \text{if} \quad |x| \geq a \end{cases}$$

where the ground state is given by :

$$E_0 = \frac{\hbar^2}{2m}\frac{\pi^2}{4a^2} \tag{1}$$

We propose to seek an approximate value of the ground state energy by the variational method. To this end, we consider the functions :

$$\psi_\lambda(x) = \begin{cases} a^\lambda - |x|^\lambda & \text{si} \quad |x| < a \\ 0 & \text{si} \quad |x| \geq a \end{cases} \tag{2}$$

We recall that the condition $\lambda > 1$ is imposed because the derivative of a wavefunction is generally continuous at all points where the potential is continuous (or has only a finite jump).

1. Calculate $\langle\psi_\lambda|\psi_\lambda\rangle$.

   We start by calculating $\langle\psi_\lambda|\psi_\lambda\rangle$:

$$\langle\psi_\lambda|\psi_\lambda\rangle = \int_{\mathbb{R}} |\psi_\lambda(x)|^2 \mathrm{d}x = \int_{-a}^{a} \left(a^\lambda - |x|^\lambda\right)^2 \mathrm{d}x \qquad (y \in \mathbb{R} \implies |y|^2 = y^2)$$

$$= 2\int_0^a \left(a^\lambda - x^\lambda\right)^2 \mathrm{d}x \tag{3}$$

$$= 2\left(a^{2\lambda+1} - 2a^\lambda \frac{a^{\lambda+1}}{\lambda+1} + \frac{a^{2\lambda+1}}{2\lambda+1}\right) = 4a^{2\lambda+1}\frac{\lambda^2}{(\lambda+1)(2\lambda+1)} \tag{4}$$

2. Determine the value of λ that minimizes the energy. Compare with the exact ground state energy and deduce the relative error.

Solution : Calculate first :

$$\begin{aligned}
\langle\psi_\lambda|H|\psi_\lambda\rangle &= \int_{\mathbb{R}} \psi_\lambda^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{\mathrm{d}x^2}+V(x)\right)\psi_\lambda(x)\mathrm{d}x \\
&= -\frac{\hbar^2}{2m}2\int_0^a\left(a^\lambda - x^\lambda\right)\frac{d^2}{\mathrm{d}x^2}\left(a^\lambda - x^\lambda\right)\mathrm{d}x \\
&= \frac{\hbar^2}{2m}2\int_0^a\left(a^\lambda - x^\lambda\right)\lambda(\lambda-1)x^{\lambda-2}\mathrm{d}x \\
&= \frac{\hbar^2}{2m}2\left(a^\lambda\lambda(\lambda-1)\frac{a^{\lambda-1}}{\lambda-1} - \lambda(\lambda-1)\frac{a^{2\lambda-1}}{2\lambda-1}\right) \\
&= \frac{\hbar^2}{m}a^{2\lambda-1}\frac{\lambda^2}{2\lambda-1} \qquad (5)
\end{aligned}$$

With (4) and (5), we can calculate the energy of the state $|\psi_\lambda\rangle$:

$$E_{\text{var}}(\lambda) = \frac{\langle\psi_\lambda|H|\psi_\lambda\rangle}{\langle\psi_\lambda|\psi_\lambda\rangle} = \frac{\hbar^2}{m}\frac{1}{4a^2}\frac{(\lambda+1)(2\lambda+1)}{2\lambda-1} = \frac{\hbar^2}{m}\frac{1}{4a^2}\frac{2\lambda^2+3\lambda+1}{2\lambda-1} \qquad (6)$$

The minimum energy is therefore achieved for the value of λ that minimizes $\frac{2\lambda^2+3\lambda+1}{2\lambda-1}$. To calculate this λ, we set :

$$0 = \frac{\partial}{\partial\lambda}\frac{2\lambda^2+3\lambda+1}{2\lambda-1} = \frac{(4\lambda+3)(2\lambda-1)-2(2\lambda^2+3\lambda+1)}{(2\lambda-1)^2} = \frac{(4\lambda^2-4\lambda-5)}{(2\lambda-1)^2}$$

By requiring that the numerator vanishes, we find the roots $\lambda_{+,-} = \frac{1\pm\sqrt{6}}{2}$, and since we want $\lambda > 1$, we keep the positive root :

$$\lambda_+ = \frac{1+\sqrt{6}}{2} \approx 1.72$$

As the function $\frac{2\lambda^2+3\lambda+1}{2\lambda-1}$ diverges as $\lambda\to\infty$, while its derivative is negative as $\lambda\to 1$, we can see that it reaches its minimum at the point λ_+. We could alternatively compute the second derivative and observe that it is positive at λ_+.

By plugging λ_+ into (6), we find :

$$E_{\text{var}}(\lambda_+) = \frac{\hbar^2}{2m}\frac{1}{4a^2}\left(5+2\sqrt{6}\right)$$

Comparing with the exact energy of the ground state :

$$E_0 = \frac{\hbar^2}{2m}\frac{\pi^2}{4a^2}$$

gives a relative error of :

$$\frac{E_{\text{var}}(\lambda_+)}{E_0} = \frac{5+2\sqrt{6}}{\pi^2} \approx 1.00298$$

So we see that our variational function - albeit very simple - gives an energy remarkably close to the exact ground state energy. Therefore, we expect $|\psi_{\lambda_+}\rangle$ to accurately describe the physics of the ground state.

Group and Representation Theory

The aim of this part of the problem sheet is just to build familiarity with the basics of groups and representation theory. There are quite a few questions but most are pretty quick and easy once you are comfortable with the basic ideas. And if this all feels pretty foreign currently getting comfortable with these ideas will be essential to follow the rest of the course.

Problem 2 : Pauli matrices for groups

1. Prove that the Pauli matrices and the identity (times $\pm 1,\ \pm i$) form a (non-Abelian) group with the matrix product.

A group has to have different properties.

- Closed : As we know $\sigma_i \sigma_j = i\epsilon_{ijk}\sigma_k$, so the product of two Pauli matrices is a Pauli matrix with a pre-factor of either $\pm 1,\ \pm i$, so the product of each of two possible matrices is in the set of our matrices.
- Associative : The matrix product is associative.
- Identity : The group includes the identity matrix.
- Inverse : we can check that $\sigma_i \sigma_i = \mathbb{1}$, $i\sigma_i \times -i\sigma_i = \mathbb{1}$, $-\mathbb{1} \times -\mathbb{1} = \mathbb{1}$. So the inverse of each matrix is in the set of our matrices as well.

2. Prove that the trace-less hermitian 2x2 matrices form a group with the matrix sum.

Equivalently we check the properties of groups, we call this set of trace-less hermitian 2×2 matrices C.

- Closeness : If $A, B \in C$, then $\text{Tr}[A+B] = 0$ so $A + B \in C$.
- Associative : The matrix sum is associative.
- Identity. We have $\text{Tr}[0] = 0$ so $0 \in C$. The group includes the 0 matrix, the identity with the sum.
- Inverse : For any matrix A, $-A$ is the inverse with the sum.

Problem 3 : Groups and the complex plane

Given $n \in \mathbb{N}$, show that the set of n-th roots of 1 (in the complex plane) form an Abelian group under the product.

The n-roots of 1 can be written as $e^{-i\frac{2\pi k}{n}}$ where $0 \leq k \leq n$. Then

- Closeness : $e^{-i\frac{2\pi k}{n}} e^{-i\frac{2\pi k'}{n}} = e^{-i\frac{2\pi(k+k')}{n}} = e^{-i\frac{2\pi \tilde{k}}{n}}$ with $\tilde{k} = k + k'$.
- Associative : The scalar product is associative.
- Identity : For $k = 0$, $e^{-i2\pi k/n} = 1$. The identity with the product
- Inverse : We want$e^{-i2\pi k/n} e^{-i2\pi k'/n} = 1$, this implies $k' = -k$ or in other words $k' = 2\pi - k$ to keep it positive.

Problem 4 : Subgroups

A subset H of the group G is a subgroup of G iff it is nonempty and itself forms a group.

1. The closure condition entails that whenever a and b are in H, then $a * b$ and a^{-1} are also in H. Show that these two conditions can be combined into one equivalent condition : whenever a and b are in H, then $a * b^{-1}$ is also in H.

The statements are

(A) "*whenever a and b are in H, then $a * b$ and a^{-1} are also in H*"
(B) "*whenever a and b are in H, then $a * b^{-1}$ is also in H*"

To be *equivalent*, we must prove (A) implies (B) *and* (B) implies (A).

We begin with (A) $\implies$ (B). We can show this by taking $a * b$ and a^{-1} which are in the group. Now take $b = a^{-1}$, so we have $a * a^{-1} = e$ is also in the group. Now we can write $a * b = e \in H$ and then we have $a = b^{-1}$ is also in the group. So finally we have $a * b^{-1} \in H$. By symmetry if b and a are in H, then $b * a$ and b^{-1} are also in H. Then consider a and b^{-1} that are in H we have $a * b^{-1}$ that is also in H

We now show (B) $\implies$ (A). We know that for each a and b in H we have $a * b^{-1} \in H$. Since H is not empty we can take $a = b$ and then we have $a * a^{-1} = e \in H$. Now we can take this identity element and write $e * a^{-1} \in H$,by taking e and b in H, which gives us that the inverse element is also in H. Finally if we take a and b^{-1} we have $a * b \in H$.

2. Explain how this condition can be used to help identify subgroups.

From the previous part, we can see that the necessary and sufficient condition for a subset H of a group G to be a subgroup of that group is for each a and b in a subset we have $a * b^{-1} \in H$. From this, we can say that to identify a subgroup we can check if $HH^{-1} = H$. In the case that we have $HH^{-1} = H$, H is a subgroup of G.

Problem 5 : Building basic familiarity with tensor products and direct sums

1. Let $M_1 = \sigma_x \oplus \sigma_x$. Write the matrix explicitly and find the eigenstates (you do not need to diagonalize the matrix).

$$M_1 = \begin{pmatrix} \sigma_x & 0_{2\times 2} \\ 0_{2\times 2} & \sigma_x \end{pmatrix} \tag{7}$$

We know that we have $(A \oplus B)(|x\rangle \oplus |y\rangle) = (A|x\rangle) \oplus (B|y\rangle)$. So we can use the eigenstates and eigenvalues of σ_x to find the eigenstates of the $\sigma_x \oplus \sigma_x$. The eigenstates are $\{|+\rangle \oplus 0, |-\rangle \oplus 0, 0 \oplus |+\rangle, 0 \oplus |-\rangle\}$. Note that here 0 is the actual 0-vector, not to be confused with $|0\rangle$

2. Let $M_1' = \mathbb{1} \otimes \sigma_x$. Write the matrix explicitly and find the eigenstates (you do not need to diagonalize the matrix).

$$M_1' = \begin{pmatrix} \sigma_x & 0_{2\times 2} \\ 0_{2\times 2} & \sigma_x \end{pmatrix} \tag{8}$$

The eigenstates are $\{|0\rangle \otimes |+\rangle, |0\rangle \otimes |-\rangle, |1\rangle \otimes |+\rangle, |1\rangle \otimes |-\rangle\}$.

3. Is it a coincidence that $M_1 = M_1'$? If it is not state why ?

Yes.

4. Now let $M_2 = \sigma_z \oplus \sigma_x$. Write the matrix explicitly and find the eigenstates (you do not need to diagonalize the matrix).

$$M_2 = \begin{pmatrix} \sigma_z & 0_{2\times 2} \\ 0_{2\times 2} & \sigma_x \end{pmatrix} \tag{9}$$

We know that we have $(A \oplus B)(|x\rangle \oplus |y\rangle) = (A|x\rangle) \oplus (B|y\rangle)$. So we can use the eigenstates and eigenvalues of σ_z and σ_x to find the eigenstates of the $\sigma_z \oplus \sigma_x$. The eigenstates are $\{0 \oplus |+\rangle, 0 \oplus |-\rangle, |0\rangle \oplus 0, |1\rangle \oplus 0\}$.

5. And let $M_2' = \sigma_z \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_x$. Write the matrix explicitly.

$$M_2' = \begin{pmatrix} \mathbb{1} & 0_{2\times 2} \\ 0_{2\times 2} & -\mathbb{1} \end{pmatrix} + \begin{pmatrix} \sigma_x & 0_{2\times 2} \\ 0_{2\times 2} & \sigma_x \end{pmatrix} = \begin{pmatrix} \mathbb{1} + \sigma_x & 0_{2\times 2} \\ 0_{2\times 2} & -\mathbb{1} + \sigma_x \end{pmatrix} \tag{10}$$

6. Is it true that $M_2 = M_2'$?

They are not equal

7. Using the commutation relationships of the Pauli matrices find the commutation relationships of $\sigma_i \otimes \sigma_j$ where $i, j \in \{x, y, z\}$.

For Pauli matrices, we have $[\sigma_i, \sigma_j] = 2\varepsilon_{ijk}\sigma_k$ where $i, j \in \{x, y, z\}$. Now we can use this relationship to find the commutation relationship of the tensor product of Pauli matrices.

$$[\sigma_i \otimes \sigma_j, \sigma_k \otimes \sigma_l] = (\sigma_i \otimes \sigma_j)(\sigma_k \otimes \sigma_l) - (\sigma_k \otimes \sigma_l)(\sigma_i \otimes \sigma_j) \tag{11}$$

Now to simplify this equation we use the properties of tensor products. We know that $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$. Here we rewrite the commutation.

$$[\sigma_i \otimes \sigma_j, \sigma_k \otimes \sigma_l] = (\sigma_i\sigma_k) \otimes (\sigma_j\sigma_l) - (\sigma_k\sigma_i) \otimes (\sigma_l\sigma_j) \tag{12}$$

For each of these terms, we can use $\sigma_i\sigma_j = \delta_{ij}\mathbb{1} + i\varepsilon_{ijk}\sigma_k$ and write :

$$(\sigma_i\sigma_k) \otimes (\sigma_j\sigma_l) = (\delta_{ik}\mathbb{1} + i\varepsilon_{ikk'}\sigma_{k'}) \otimes (\delta_{jl}\mathbb{1} + i\varepsilon_{jll'}\sigma_{l'}) \tag{13}$$

$$= \delta_{ik}\delta_{jl}\mathbb{1} + i\varepsilon_{ikk'}\delta_{jl}(\sigma_{k'} \otimes \mathbb{1}) + i\varepsilon_{jll'}\delta_{ik}(\mathbb{1} \otimes \sigma_{l'}) - \varepsilon_{ikk'}\varepsilon_{jll'}(\sigma_{k'} \otimes \sigma_{l'}) \tag{14}$$

In $(\sigma_k\sigma_i) \otimes (\sigma_l\sigma_j)$ we just need to permute i with k and j with l. As the first and last terms are symmetric under this permutation they will cancel each other In the end, we have

$$[\sigma_i \otimes \sigma_j, \sigma_k \otimes \sigma_l] = 2i\varepsilon_{ikk'}\delta_{jl}(\sigma_{k'} \otimes \mathbb{1}) + 2i\varepsilon_{jll'}\delta_{ik}(\mathbb{1} \otimes \sigma_{l'}) \tag{15}$$

8. Now find the commutation relationships of $\sigma_i \oplus \sigma_j$. Why are these different ?

We want to find the commutation relationship of the direct sum of Pauli matrices.

$$[\sigma_i \oplus \sigma_j, \sigma_k \oplus \sigma_l] = (\sigma_i \oplus \sigma_j)(\sigma_k \oplus \sigma_l) - (\sigma_k \oplus \sigma_l)(\sigma_i \oplus \sigma_j) \tag{16}$$

To calculate this commutator, we use the property of direct sums and commutators. The direct sum of matrices $A \oplus B$ and $C \oplus D$ is defined as :

$$A \oplus B = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}$$

$$C \oplus D = \begin{pmatrix} C & 0 \\ 0 & D \end{pmatrix}$$

The commutator $[A \oplus B, C \oplus D]$ is then :

$$[A \oplus B, C \oplus D] = (A \oplus B)(C \oplus D) - (C \oplus D)(A \oplus B)$$

Expanding this product, we get :

$$(A \oplus B)(C \oplus D) = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & D \end{pmatrix} = \begin{pmatrix} AC & 0 \\ 0 & BD \end{pmatrix}$$

$$(C \oplus D)(A \oplus B) = \begin{pmatrix} C & 0 \\ 0 & D \end{pmatrix} \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} = \begin{pmatrix} CA & 0 \\ 0 & DB \end{pmatrix}$$

Thus, the commutator is :

$$[A \oplus B, C \oplus D] = \begin{pmatrix} AC & 0 \\ 0 & BD \end{pmatrix} - \begin{pmatrix} CA & 0 \\ 0 & DB \end{pmatrix} = \begin{pmatrix} [A, C] & 0 \\ 0 & [B, D] \end{pmatrix}$$

Applying this to our specific case with Pauli matrices $\sigma_i \oplus \sigma_j$ and $\sigma_k \oplus \sigma_l$:

$$[\sigma_i \oplus \sigma_j, \sigma_k \oplus \sigma_l] = \begin{pmatrix} [\sigma_i, \sigma_k] & 0 \\ 0 & [\sigma_j, \sigma_l] \end{pmatrix}$$

Given that the commutator of Pauli matrices σ_i and σ_k (where $i, k \in \{x, y, z\}$) is :

$$[\sigma_i, \sigma_k] = 2i\epsilon_{ijk}\sigma_j$$

where ϵ_{ijk} is the Levi-Civita symbol, we have :

$$[\sigma_i, \sigma_k] = 2i\epsilon_{ikm}\sigma_m$$

$$[\sigma_j, \sigma_l] = 2i\epsilon_{jln}\sigma_n$$

Thus, the commutator of the direct sum of Pauli operators is :

$$[\sigma_i \oplus \sigma_j, \sigma_k \oplus \sigma_l] = \begin{pmatrix} 2i\epsilon_{ikm}\sigma_m & 0 \\ 0 & 2i\epsilon_{jln}\sigma_n \end{pmatrix}$$

Problem 6 : Tensor products and direct product representations

Show that if $R(g)$ is a representation to a group G then $R(g)^{\otimes k}$ and $\bigoplus_k R(g)$ are also representations for G.

We start by assuming we have the map $R : G \to GL(V)$ that brings the group to a representation. Then, if R is a homomorphism, it means that the map $R_k : G \to GL(V)^{\otimes k}$ and the map $\tilde{R}_k : G \to \oplus_k GL(V)$ are a homomorphism as well. To prove it we use the definition of a homomorphism, $R(g * h) = R(g) \times R(h)$ for $g, h \in G$.

To prove that $R(g)^{\otimes k} = R(g) \otimes ... \otimes R(g)$ is a homomorphism we have to show that $R(g*h)^{\otimes k} = R(g)^{\otimes k} \times R(h)^{\otimes k}$.

$$R(g*h)^{\otimes k} = R(g*h) \otimes ... \otimes R(g*h) = R(g) \times R(h) \otimes ... \otimes R(g) \times R(h) \tag{17}$$
$$= R(g) \otimes ... \otimes R(g) \times R(h) \otimes ... \otimes R(h) = R(g)^{\otimes k} \times R(h)^{\otimes k} \tag{18}$$

Here we use the property of tensor product $(AC) \otimes (BD) = (A \otimes B)(C \otimes D)$
Then to prove that $\bigoplus_k R(g) = (R \bigoplus ... \bigoplus R)(g) = (R(g), ..., R(g))$ is a homomorphism we have to show that $\bigoplus_k R(g*h) = \bigoplus_k R(g) \times \bigoplus_k R(h)$.

$$\bigoplus_k R(g*h) = (R \bigoplus ... \bigoplus R)(g*h) = (R(g*h), ..., R(g*h)) \tag{19}$$
$$= (R(g) \times R(h), ..., R(g) \times R(h)) = (R(g), ..., R(g)) \times (R(h), ..., R(h)) \tag{20}$$
$$= \bigoplus_k R(g) \times \bigoplus_k R(h) \tag{21}$$

Here we use the block structure of $(R(g) \times R(h), ..., R(g) \times R(h))$ to use only one matrix multiplication.

Problem 7 : The regular representation

For a finite group of order h, one can construct the so-called regular representation using $h \times h$ matrices as follows. First start from the following *reordered* Cayley table (here for $h = 3$) :

$$C = \begin{array}{c|ccc} * & e & a^{-1} & b^{-1} \\ \hline e & e & a^{-1} & b^{-1} \\ a & a & e & ab^{-1} \\ b & b & ba^{-1} & e \end{array} \tag{22}$$

Now the representation can be done using the following matrices for $g \in G$: We use a matrix which is zero everywhere except for the position that corresponds to the group element in the Cayley table :

$$(R(g))_{ij} = \delta_{g,C_{ij}} \tag{23}$$

1. Deduce the regular representation for $\mathbb{Z}_3$. Verify that it is indeed a representation of $\mathbb{Z}_3$

To find the regular representation of $\mathbb{Z}_3 = \{e, a, b\}$, we start by finding its reordered Cayley table.

$$C = \begin{array}{c|ccc} * & e & a^{-1} & b^{-1} \\ \hline e & e & b & a \\ a & a & e & b \\ b & b & a & e \end{array} \tag{24}$$

Now we have the representation of each group element.

$$R(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{25}$$

$$R(a) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{26}$$

$$R(b) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \tag{27}$$

If we check, we can see that with this representation we have all the properties of a group. It can be done simply by checking if for every a and b in $\mathbb{Z}_3$ we have $R(a * b) = R(a) * R(b)$

2. What about $\mathbb{Z}_n$?

We can also consider the cyclic group of n objects. From the lecture notes we had the Cayley table of $\mathbb{Z}_n$ which is as follows.

$$\begin{array}{c|cccccc} * & e & a_1 & a_2 & \dots & a_n \\ \hline e & e & a_1 & a_2 & \dots & a_n \\ a_1 & a_1 & a_2 & a_3 & \dots & e \\ a_2 & a_2 & a_3 & a_4 & \dots & a_1 \\ \vdots & & & & & \\ a_n & a_n & e & a_1 & \dots & a_{n-1} \end{array} \tag{28}$$

From this table, we can see that if we find the regular representation, it would be just a representation. In other words, if we consider our group elements as $\{e, a, a^2, \dots, a^{n-1}\}$ the representation of each element can be found by a permutation matrix.

$$R(a) = \begin{pmatrix} 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{pmatrix} \tag{29}$$

So we can write the representation of other elements as other permutation matrices.

$$R(a^m) = R^m(a) \tag{30}$$

And again, similar to the first part of the question, we can show that for every g_1 and g_2 in $\mathbb{Z}_n$ we have $R(g_1 * g_2) = R(a^i * a^j) = R(a^{i+j}) = R^{i+j}(a) = R^i(a)R^j(a) = R(a^i)R(a^j) = R(g_1)R(g_2)$

3. Prove that the regular representation of a group G is indeed a representation of a group G.

We know that to show if the map R is a representation or not we need to show that for each g_1 and g_2 in G we have $R(g_1 * g_2) = R(g_1) \times R(g_2)$, with $\times$ the matrix multiplication. For the regular representation, from the definition in the question we have $(R(g))_{ij} = \delta_{g,C_{ij}}$. Also, we know that in the Cayley table and at the position i, j we have the result for $g_i * g_j$. So, we should show that for each g_1 and g_2 in G,

$$(R(g_1 * g_2))_{ij} = \sum_k R(g_1)_{ik} R(g_2)_{kj} \tag{31}$$

To show that, we start with

$$(R(g_1 * g_2))_{ij} = \delta_{(g_1 g_2),C_{ij}} = \delta_{g_1 g_2, g_i g_j} = \sum_k \delta_{g_1, g_i g_k} \delta_{g_2, g_k g_j} = \sum_k \delta_{g_1, C_{ik}} \delta_{g_2, C_{kj}} \tag{32}$$

$$= \sum_k R(g_1)_{ik} R(g)_{kj} \tag{33}$$

<u>Problem 8 :</u> One of our favorite examples : the C3v group

1. Show that S_3 and C3v are isomorphic. (Does this make physical sense ?)

If we look at the definition of $S_3 = \{I, \mathrm{SWAP}_{12}, \mathrm{SWAP}_{13}, \mathrm{SWAP}_{23}, \mathrm{CYCLE}_{123}, \mathrm{CYCLE}_{321}\}$, and we construct the Cayley table, we find that is the same as for C3v. Thus they are isomorphic.

$$\begin{array}{c|cccccc} * & e & a & a^2 & b & c & d \\ \hline e & e & a & a^2 & b & c & d \\ a & a & a^2 & e & c & d & b \\ a^2 & a^2 & e & a & d & b & c \\ b & b & d & c & e & a^2 & a \\ c & c & b & d & a & e & a^2 \\ d & d & c & b & a^2 & a & e \end{array} \tag{34}$$

2. What are the subgroups for C3v ? (Does this make physical sense ?)

The Cayley table is

$$\begin{array}{c|cccccc} * & e & a & a^2 & b & c & d \\ \hline e & e & a & a^2 & b & c & d \\ a & a & a^2 & e & c & d & b \\ a^2 & a^2 & e & a & d & b & c \\ b & b & d & c & e & a^2 & a \\ c & c & b & d & a & e & a^2 \\ d & d & c & b & a^2 & a & e \end{array} \tag{35}$$

Here we can identify that $\{e, a, a^2\}$ form a subgroup as well as $\{e, b\}$, $\{e, c\}$, $\{e, d\}$.

3. Write down a representation of C3v on $\mathbb{R}^3$

4. Hence write a representation of C3v which describes the set of 3 balls in a triangle connected by springs connected shown in Fig. 1. That is, find the 6D representation describing the symmetry properties of coordinates $x_1, y_1, x_2, y_2, x_3, y_3$ of the 3 balls on the springs.

To find 6D representations you can assume the vector $v = (x_1, y_1, x_2, y_2, x_3, y_3)$ which correspond to the position of the balls. What the transformation will do is, first ,to exchange the balls, and then to physically perform either a rotation or a symmetry on the ball itself! In other words, the 6D representation can be written as

$$D^{6D} = D^{3D} \otimes D^{2D} \tag{36}$$

We first try to find the representation of C3v in 2D. To find them you can think of the isometry of an equilateral triangle in a 2D space , a and a^2 are the rotations of $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$ around it's centre and b, c and d are the reflection around each symmetry axis of the triangle.

The representations on $\mathbb{R}^2$ are the following matrices

$$e = \begin{pmatrix} 1, 0 \\ 0, 1 \end{pmatrix}, a = \begin{pmatrix} -\frac{1}{2}, -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2}, -\frac{1}{2} \end{pmatrix}, a^2 = \begin{pmatrix} -\frac{1}{2}, \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2}, -\frac{1}{2} \end{pmatrix}, \tag{37}$$

$$b = \begin{pmatrix} -1, 0 \\ 0, 1 \end{pmatrix}, c = \begin{pmatrix} \frac{1}{2}, \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2}, -\frac{1}{2} \end{pmatrix}, d = \begin{pmatrix} \frac{1}{2}, -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2}, -\frac{1}{2} \end{pmatrix} \tag{38}$$

Then we find the representation of C3v in 3D. Here we can think of an triangle in a 3D space with vertex at positions (1 ;0 ;0), (0 ;1 ;0) and (0 ;0 ;1). Now you can think of each isometry as an exchange in the position of the vertex.

$$e = \begin{pmatrix} 1,0,0 \\ 0,1,0 \\ 0,0,1 \end{pmatrix}, a = \begin{pmatrix} 0,0,1 \\ 1,0,0 \\ 0,1,0 \end{pmatrix}, a^2 = \begin{pmatrix} 0,1,0 \\ 0,0,1 \\ 1,0,0 \end{pmatrix}, \tag{39}$$

$$b = \begin{pmatrix} 1,0,0 \\ 0,0,1 \\ 0,1,0 \end{pmatrix}, c = \begin{pmatrix} 0,0,1 \\ 0,1,0 \\ 1,0,0 \end{pmatrix}, d = \begin{pmatrix} 0,1,0 \\ 1,0,0 \\ 0,0,1 \end{pmatrix} \tag{40}$$

You will then end up with 6×6 matrix that you can find in Florent Krzakala's notes in part 5.5 on Moodle.

5. Write down the regular representation of the group.

To obtain the regular representation, we have to use the reordered Cayley table where we only have the identity element e in the diagonal

$*$	e	a	a^2	b	c	d
e	e	a	a^2	b	c	d
a^2	a^2	e	a	d	b	c
a	a	a^2	e	c	d	b
b	b	d	c	e	a^2	a
c	c	b	d	a	e	a^2
d	d	c	b	a^2	a	e

(41)

Then we can find the matrix

$$R(e) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \tag{42}$$

$$R(a) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \tag{43}$$

You can continue this and find $R(b)$, $R(c)$, and $R(d)$.

<u>Problem 9 :</u> Continuous groups and their representations

Consider the following continuous groups : $U(1)$, $U(2)$, $SU(2)$, $O(3)$. In each case :

1. Describe a physical system with this symmetry.

— $U(1)$ The phase of a laser.

— $U(2)$ Light polarisation

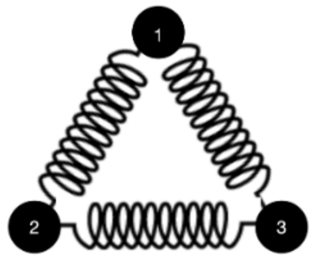

FIGURE 1 – Three balls in a triangle connected by springs.

— $SU(2)$ Qubit.
— $O(3)$ 3-d rotations.

2. Write down a representation for the group.

— $U(1) \to e^{-i\phi}$
— $U(2) \to e^{-i\phi}e^{-i\sigma_x\theta_1}e^{-i\sigma_z\theta_2}e^{-i\sigma_x\theta_3}$
— $SU(2) \to e^{-i\sigma_x\theta_1}e^{-i\sigma_z\theta_2}e^{-i\sigma_x\theta_3}$
— $O(3) \to e^{-iL_x\theta_1}e^{-iL_y\theta_2}e^{-iL_x\theta_3}$, where L_i are the angular momentum generators for the direction i.

3. Does the group have any finite subgroups ? (Give examples or explain why there are not any.)

All of them do. Here some examples

— $U(1)$, the $n-$th roots of 1, for a given n.
— $U(2)$ we see that we can define $e^{-i\sigma_x\pi}$ and this and $\mathbb{1}$ form a finite subgroup.
— $SU(2)$ the same as for $U(2)$.
— $O(3)$ making, again, a rotation proportional to π and not making this rotation on one axis of $3-d$ space, is a finite subgroup.

4. Does the group have any continuous subgroups ? (Give examples or explain why there are not any.)

All of them except for the $U(1)$ group have subgroups. $SU(2)$ is a subgroup of $U(2)$, $e^{-i\sigma_z x}$ is a subgroup for all x of $SU(2)$. Rotations along one axis are one subgroup of $O(3)$.