Quantum mechanics II, Problems 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:

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

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:

$$\psi_{\lambda}(x) = \begin{cases} a^{\lambda} - |x|^{\lambda} & \text{if } |x| < a \\ 0 & \text{if } |x| \ge a \end{cases}$$
 (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 $\langle \psi_{\lambda} | \psi_{\lambda} \rangle$.
- 2. Determine the value of λ that minimizes the energy. Compare with the exact ground state energy and deduce the relative error.

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 ± 1 , $\pm i$) form a (non-Abelian) group with the matrix product.
- 2. Prove that the trace-less hermitian 2x2 matrices form a group with the matrix 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.

Problem 4 : Subgroups

A subset $H \subseteq G$ 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.
- 2. Explain how this condition can be used to help identify subgroups.

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).
- 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).
- 3. Is it a coincidence that $M_1 = M'_1$? If it is not state why?
- 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).
- 5. And let $M_2' = \sigma_z \otimes \mathbb{1} + \mathbb{1} \otimes \sigma_x$. Write the matrix explicitly.
- 6. Is it true that $M_2 = M_2'$?

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.

Problem 7: The C3v group

- 1. Show that S_3 and C_3 v are isomorphic. (Does this make physical sense?)
- 2. What are the subgroups for C3v? (Does this make physical sense?)
- 3. 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.

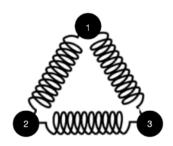


FIGURE 1 – Three balls in a triangle connected by springs.

Problem 8: Continuous groups and their representations

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

- 1. Name a physical system that is described by this group.
- 2. Write down a representation for the group.
- 3. Does the group have any finite subgroups? (Give examples or explain why there are not any.)
- 4. Does the group have any continuous subgroups? (Give examples or explain why there are not any.)