Quantum mechanics II, Problems 8 - Irreps

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Problem 1 : Warm up : Irreps of two qubits

Consider a representation U_g of $SU(2)$. Now consider the representation of the tensor product

$$R(g) = U_g \otimes U_g \tag{1}$$

can we decompose this in the direct sum of two representations ? That is, can you find the irreductible representations of this ?

Problem 2 : Irreps of the Cyclic group

The aim here is to become familiar with the irreducible representations of the cyclic group.

1. Show that all irreducible representations of an Abelian group are of dimension $n_j = 1$.
2. Consider the cyclic group $Z_3 = \{e, a, b\}$ of order 3. Recall its multiplication table.
3. There are 3 irreducible representations for $Z_3 = \{e, a, b\}$ group. What dimension are they ?
4. Compute the irreducible representations for $Z_3 = \{e, a, b\}$. Verify that these representations are indeed irreducible.

   Hint : recall Schur's Theorem.
5. There are n irreducible representations for Z_n group. Compute these representations and their dimension.

Problem 3 : Irreps of C_{3v}

The aim of this exercise is to consider two representations of the group C_{3v}. We will start by finding the representation R of the group on the vector space $\mathbb{R}^2$. Then we will find the representation P_R of the group on the function space generated by $\Psi_1(\mathbf{r}) = x^2 e^{-r}$, $\Psi_2(\mathbf{r}) = y^2 e^{-r}$, $\Psi_3(\mathbf{r}) = 2xye^{-r}$. We will show that the representation P_R is reducible. We will establish the connection with the representation R of dimension 2.

1. Consider the vector space $\mathbb{R}^2$ with vectors (x, y). Derive the representation of $R(\sigma_1)$ and $R(C_3)$ in this space. Then deduce the group multiplication table to find $R(u)$, $\forall u \in C_{3v}$. We will assume that this representation is unitary and irreducible, which can be demonstrated by Schur's theorem.

2. Consider now the vector space of functions $\mathcal{H}$, generated by functions :

$$\Psi_1(\mathbf{r}) = x^2 e^{-r}$$
$$\Psi_2(\mathbf{r}) = y^2 e^{-r}$$
$$\Psi_3(\mathbf{r}) = 2xye^{-r}$$

where $r = |\mathbf{r}| = \sqrt{x^2 + y^2}$, with the scalar product :

$$\langle \Psi_\alpha | \Psi_\beta \rangle = \int d^2\mathbf{r} \Psi^*_\alpha(\mathbf{r}) \Psi_\beta(\mathbf{r}).$$

Written as matrices, the group representation C_{3v} is defined as follows :

$$P_{R(u)} \Psi(\mathbf{r}) \equiv \Psi(R^{-1}(u)\mathbf{r}), \; \forall u \in \mathcal{H},$$

where $R(u)$ are the matrices derived in point (a) (in quantum mechanics, for example, the wave function of a particle obeys this transformation law following a rotation of the reference frame). Show that it is a representation of the group, and that its matrices are not all unitary.

3. Show that the representation $R(u)$ is reducible by identifying an invariant subspace.
4. Hence show that the representation $R(u)$ can be written as a direct sum of a 2D and 1D irreducible representations.

Problem 4 : Particle in a periodic potential

Consider Hamiltonian $1D$:

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial \hat{x}^2} + \hat{V}(\hat{x})$$

where $V(x)$ is a periodic potential of period a, ie :

$$V(x + a) = V(x).$$

Suppose that the system is confined to a region of width $L = la$ (periodic boundary conditions), where l is a positive integer. The aim of this exercise is to find what can be said on the form of the eigenfunctions of $\hat{H}$ by using the symmetries of the problem.

1. Find the symmetry group G of $\hat{H}$ and write the l irreducible representations of this group.
2. Determine the transformation law of the eigenfunctions of $\hat{H}$ under the transformations of the symmetry group G.
3. Show that the eigenfunctions of $\hat{H}$ are of the form :

   $$\psi_k(x) = u_k(x) e^{ikx} \quad (k = 2\pi n/L, \; n = 1, 2, ..., l).$$

   where the functions $u_k(x)$ are periodic with period a. This result is, in one dimension, the Bloch theorem for electronic states in a crystal.
4. (**non-examinable**) Suppose that the potential $V(x)$ has the form $V(x) = \sum_{n=0}^{l-1} u(x - na)$, where $u(x)$ is a deep potential well. The total potential $V(x)$ is then a "chain" of potential wells. (recall that, due to the use of periodic boundary conditions, the coordinates x and $x - la$ coincide). Assume that the ground state of a single-well has wavefunction $\varphi_0(x)$ and energy ϵ_0, so that

   $$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + u(x) \right] \varphi_0(x) = \epsilon_0 \varphi_0(x) \; .$$

   Within the tight-binding approximation, we can assume that the lowest energy states of the full problem, with the chain potential $V(x) = \sum_{n=0}^{l-1} u(x - na)$ are given approximately by linear combinations of the "atomic" ground state orbitals localized at the different wells : $\psi_k(x) = \sum_{n=0}^{l-1} C_{k,n} \varphi_0(x - na)$. This approximation is justified by the fact that, when the potential wells are very deep, the wavefunctions of the lowest states must be composed mostly of the lowest atomic states and not of the excited levels of a single well.

   (a) What is the Bloch wavefunction u_k assuming the tight-binding approximation ?
   (b) Calculate the average energy of the state $\psi_k = u_k \mathrm{e}^{ikx}$ in the tight-binding approximation ?