Quantum mechanics II, Problems 8 : Irreps

Solutions

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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 irreducible representations of this ?
Notice that this tensor product commutes with the SWAP gate $[U_g \otimes U_g, \text{SWAP}] = 0$. This means that is possible to block diagonalise $U_g \otimes U_g$ in the same basis as the SWAP.

We can deduce (or recall) that the symmetric space has eigenvalue 1 for the SWAP operator. That is

$$\text{SWAP} |00\rangle = |00\rangle \tag{2}$$

$$\text{SWAP} |11\rangle = |11\rangle \tag{3}$$

$$\text{SWAP} \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) \tag{4}$$

However, the antisimetric space has eigenvalue -1. That is

$$\text{SWAP} \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) = -\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) \tag{5}$$

Therefore, this means that $U_g \otimes U_g$ can be block diagonalised by the symmetric-antisymmetric decomposition.
Notice that this is only valid for the representation of a spin-$\frac{1}{2}$. If we take the spin-1 representation of SU(2), $R(g)$ will be a 9 dimensional representation and the permutation with SWAP will not be enough to fully reduce the representation.
However, we can write down the general decomposition into irreducible representations using Clebsch Gordon theory. First note that the irreducible representations of SU(2) of dimension d are the spin-representations (e.g. the spin-1/2 representation is given by the pauli matrices etc.). Lets denote this representation by $U_{1/2}$. Then we have by Clebsch Gordon :

$$U_{1/2} \otimes U_{1/2} = U_1 \oplus U_0 \tag{6}$$

You can see this by looking at the possible states that you obtain from summing two spin-1/2 :

1. Spins are aligned : The total spin is 1 and you have three different projections onto the z-axis : $m = 0, \pm 1$.
2. Spins are anti aligned : The total spin is 0 and you have one possible projection $m = 0$.

The first case above corresponds to the irreducible representation of spin-1 : U_1, while the latter corresponds to the spin-0 representation U_0.

For two irreducible representations U_{l_1}, U_{l_2} we have :

$$U_{l_1} \otimes U_{l_2} = \bigoplus_{i=|l_1-l_2|}^{l_1+l_2} U_i \tag{7}$$

.

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 $n_j = 1$.
   Suppose, for the sake of contradiction, that there exists an irreducible representation R_i of dimension $d \neq 1$. We know that there is at least one element of the group $y \in H$ that is represented by a non-diagonal matrix $R(y)$. Indeed, if all elements are diagonal, then the dimension of the representation is not appropriate and can be reduced to 1. Moreover, the group H is abelian, so we have the property :

   $$R(x)R(y) = R(x \star y) = R(y \star x) = R(y)R(x), \forall x \in H \tag{8}$$

   and for Schur's Lemma, this implies that $R(y) = \lambda \mathbb{1}$, contradicting the initial assumption.
2. Consider the cyclic group $Z_3 = \{e, a, b\}$ of order 3. Recall its multiplication table.
   The multiplication table of Z_3 is constructed very easily by filling in the trivial first rows and columns. The remaining 4 elements are immediately found by respecting the cyclicity of the group $a^3 = e$:

	e	a	a^2
e	e	a	a^2
a	a	a^2	e
a^2	a^2	e	a

3. There are 3 irreducible representations for $Z_3 = \{e, a, b\}$ group. What dimension are they ?
   As the cyclic group Z_3 is also Abelian we know from question 1 that every irreducible representations are of dimension 1.
   Here the number of irreducible representations was given, but if you were asked to find the number of irreducible representations, you should have used Burnside lemma. From question 1 we know that all irreducible representation are of dimension 1. Then using Burnside lemma and as as Z_3 is a group of order 3 we have

   $$\sum_{a=1}^{n} 1^2 = 3 \tag{9}$$

   and we can deduce that n =3. So there is 3 irreducible representations.
4. Compute the irreducible representations for $Z_3 = \{e, a, b\}$. Verify that these representations are indeed irreducible.
   Hint : recall Schur's Theorem.
   The first irreducible representation R^0 is the trivial representation $R^0(e) = 1$, $R^0(a) = 1$,

$R^0(a^2) = 1$. The two other irreducible representations are based on the cube root of unity, $e^{\frac{2\pi i}{3}}$ and $e^{\frac{4\pi i}{3}}$. R^1 will be $R^1(e) = 1$, $R^1(a) = e^{\frac{2\pi i}{3}}$ and $R^1(a^2) = e^{\frac{4\pi i}{3}}$, and R^2 will be $R^2(e) = 1$, $R^2(a) = e^{\frac{4\pi i}{3}}$, $R^2(a^2) = e^{\frac{2\pi i}{3}}$

To check that these representations are indeed irreducible we can use the Schur's Theorem. If we take

$$AR^0(g) = R^1(g)A \quad \forall g \in Z_3 \tag{10}$$

the only possible value of A is 0. Then these two representations are irreducible. We can do the same with

$$AR^0(g) = R^2(g)A \quad \forall g \in Z_3 \tag{11}$$

and

$$AR^1(g) = R^2(g)A \quad \forall g \in Z_3 \tag{12}$$

and we conclude that R^0, R^1 and R^2 are irreducible.

R^3 can be a bit hard to find, we can also use Schur's lemma to help us. As R^2 is 1-dimensional $R^3(e) = 1$, then we can write using R^0 and R^1 :

$$A1 = 1A \qquad A1 = R^2(a)A \qquad A1 = R^2(a^2)A$$

$$B1 = 1B \qquad Be^{\frac{2\pi i}{3}} = R^2(a)B \qquad Be^{\frac{4\pi i}{3}} = R^2(a^2)B$$

In order to have only $A = 0$ and $B = 0$ we must have $R^2(a) \neq 1$, $R^2(a) \neq e^{\frac{2\pi i}{3}}$, $R^2(a^2) \neq 1$, $R^2(a^2) \neq e^{\frac{4\pi i}{3}}$ and $[R^2(a)]^2 = R^2(a^2)$, $[R^2(a)]^3 = 1$. The only solution is then $R^2(e) = 1$, $R^2(a) = e^{\frac{4\pi i}{3}}$, $R^2(a^2) = e^{\frac{2\pi i}{3}}$.

5. What are the irreducible representations of Z_n ?

   To determine the irreducible representations of $G = Z_n$, we need to find groups of matrices satisfying the composition law of the cyclic group G. For a cyclic group, the search is very simple. In fact, it is immediate to find l non-equivalent irreducible representations of G of dimension 1, by considering that the l-th roots of unity and their powers satisfy the composition law of the cyclic group G. In particular, we consider the representation R^n, and we consider a vector $v \in V^{(n)}$ in the subspace $V^{(n)}$ relative to this representation. Then the fundamental element of the group U_a is represented by an operator whose action on v is :

$$R^n(U_a)v = e^{i2\pi n/l}v, n = 1, ..., l$$

   (the representation R^l is the trivial representation). Finally, we can use Burnside's theorem to assert that there are no other non-equivalent irreducible representations.

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 $\Psi_1(\mathbf{r}) = x^2e^{-r}$, $\Psi_2(\mathbf{r}) = y^2e^{-r}$, $\Psi_3(\mathbf{r}) = 2xye^{-r}$. 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.
Solution : The two dimensional representation of C_{3v} is given in the lecture notes as

$$\begin{aligned} e &= \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ C_3 &= \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \; C_3^2 = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\ \sigma_1 &= \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \; \sigma_2 = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}, \; \sigma_3 = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \end{aligned} \tag{13}$$

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

$$\begin{aligned} \Psi_1(\mathbf{r}) &= x^2 e^{-r} \\ \Psi_2(\mathbf{r}) &= y^2 e^{-r} \\ \Psi_3(\mathbf{r}) &= 2xy e^{-r} \end{aligned}$$

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.
Solution : We write down the transformations for σ_1 and C_3 explicitly. First, we note that the two dimensional representation above is unitary, so $|R(g)\mathbf{r}| = |\mathbf{r}|$ for all $g \in C_{3v}$. We find for the reflection σ_1

$$\begin{aligned} P_{R(\sigma_1)} \Psi_1(\mathbf{r}) &= \Psi(R^{-1}((\sigma_1)\mathbf{r}) = (-x)^2 e^{-r} = \Psi_1(\mathbf{r}), \\ P_{R(\sigma_1)} \Psi_2(\mathbf{r}) &= \Psi(R^{-1}((\sigma_1)\mathbf{r}) = y^2 e^{-r} = \Psi_2(\mathbf{r}), \\ P_{R(\sigma_1)} \Psi_3(\mathbf{r}) &= \Psi(R^{-1}((\sigma_1)\mathbf{r}) = -2xy e^{-r} = -\Psi_3(\mathbf{r}) \end{aligned}$$

and hence

$$P_{R(\sigma_1)} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{14}$$

For $R^{-1}(C_3) = R(C_3^2)$ we have $R^{-1}(C_3)\mathbf{r} = \begin{pmatrix} -\frac{1}{2}x + \frac{\sqrt{3}}{2}y \\ -\frac{\sqrt{3}}{2}x - \frac{1}{2}y \end{pmatrix}$ and hence

$$
\begin{aligned}
P_{R(C_3)}\Psi_1(\mathbf{r}) &= \left(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y\right)^2 e^{-r} = \left(\frac{1}{4}x^2 + \frac{3}{4}y^2 - 2\frac{\sqrt{3}}{4}xy\right) e^{-r} = \frac{1}{4}\Psi_1(\mathbf{r}) + \frac{3}{4}\Psi_2(\mathbf{r}) - \frac{\sqrt{3}}{4}\Psi_3(\mathbf{r}) \\
P_{R(C_3)}\Psi_2(\mathbf{r}) &= \left(-\frac{\sqrt{3}}{2}x - \frac{1}{2}y\right)^2 e^{-r} = \left(\frac{3}{4}x^2 + \frac{1}{4}y^2 + 2\frac{\sqrt{3}}{4}xy\right) e^{-r} = \frac{3}{4}\Psi_1(\mathbf{r}) + \frac{1}{4}\Psi_2(\mathbf{r}) + \frac{\sqrt{3}}{4}\Psi_3(\mathbf{r}) \\
P_{R(C_3)}\Psi_3(\mathbf{r}) &= 2\left(-\frac{1}{2}x + \frac{\sqrt{3}}{2}y\right)\left(-\frac{\sqrt{3}}{2}x - \frac{1}{2}y\right) e^{-r} = 2\left(\frac{\sqrt{3}}{4}x^2 - \frac{\sqrt{3}}{4}y^2 - 2\frac{1}{4}xy\right) e^{-r} \\
&= \frac{\sqrt{3}}{2}\Psi_1(\mathbf{r}) - \frac{\sqrt{3}}{2}\Psi_2(\mathbf{r}) - \frac{1}{2}\Psi_3(\mathbf{r}),
\end{aligned}
$$

We find the matrix representation

$$
P_{R(C_3)} = \begin{pmatrix} \frac{1}{4} & \frac{3}{4} & \frac{\sqrt{3}}{2} \\ \frac{3}{4} & \frac{1}{4} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{4} & \frac{\sqrt{3}}{4} & -\frac{1}{2} \end{pmatrix}. \tag{15}
$$

We can verify that this is indeed a representation, e.g. $(P_{R(\sigma_1)})^2 = (P_{R(C_3)})^3 = \mathbb{1}$.

3. Show that the representation R(u) is reducible by identifying an invariant subspace.

   Solution : We note that $v_1 = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$ is an eigenvector of both $P_{R(C_3)}$ and $P_{R(\sigma_1)}$ and hence the subspace spanned by v_1 is invariant under the action of the group.

4. Hence show that the representation R(u) can be written as a direct sum of a 2D and 1D irreducible representations.

   Solution : We first note that $R(u)$ acts trivially on the subspace V_1 spanned by v_1, hence the representation corresponding to this subspace is the trivial one dimensional representation. We find that $\mathcal{H} = V_1 \oplus V_2$ where V_2 is the complemented subspace to V_1 that is spanned by $v_{21} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, v_{22} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$. In this basis, we write down the matrix representations of the representation described above.

   $P_{R(\sigma_1)}v_{21} = \begin{pmatrix} 0 \\ 0 \\ -1 \end{pmatrix} = -v_{21}$ and $P_{R(\sigma_1)}v_{22} = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = v_{22}$

   $P_{R(C_3)}v_{21} = \begin{pmatrix} \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} \\ \frac{1}{2} \end{pmatrix} = -\frac{1}{2}v_{21} + \frac{\sqrt{3}}{2}v_{22}$ and $P_{R(C_3)}v_{22} = \begin{pmatrix} -\frac{1}{2} \\ \frac{1}{2} \\ -\frac{\sqrt{3}}{2} \end{pmatrix} = -\frac{\sqrt{3}}{2}v_{21} - \frac{1}{2}v_{22}$ therefore we find

$$
\left[P_{R(\sigma_1)}\right]_{V_2} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \tag{16}
$$

$$
\left[P_{R(C_3)}\right]_{V_2} = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \tag{17}
$$

which is equivalent to the two dimensional representation discussed before. Hence $R(u) = R_1(u) \oplus R_2(u)$.
Alternatively you can find the irreducible representations via block diagonalization of the original representations. If we define the change of basis matrix $V = [v_1, v_{21}, v_{22}]$ and we perform the change of basis trasformation on the original representation matrices, we find :

$$P'_{R(\sigma_1)} = VP_{R(\sigma_1)}V^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{18}$$

$$\tag{19}$$

$$P'_{R(C_3)} = VP_{R(C_3)}V^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}. \tag{20}$$

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.
   In the general case, the only symmetry transformations of $\hat{H}$ are the translations $U_a^n = (U_a)^n$ which translate the coordinate x by $-na$, where n is an integer multiple. The operator $P_{U_a^n}$ corresponding to the translation U_a^n and acting on the wave functions $\psi(x)$ is defined by :

   $$P_{U_a^n}\psi(x) = \psi(x+na).$$

   To determine the group G of these translations, it suffices to observe that, given the finite size $L = la$, the non-equivalent translations are l, and that each translation is equal to a power of the translation by a, U_a, i.e. :

   $$G = \{U_a, U_a^2, U_a^3, ...U_a^{l-1}, U_a^l = e\}.$$

   Therefore, the group G is the cyclic group of order l.
   To determine the irreducible representations of G, we need to find groups of matrices satisfying the composition law of the cyclic group G. For a cyclic group, the search is very simple. In fact, it is immediate to find l non-equivalent irreducible representations of G of dimension 1, by considering that the l-th roots of unity and their powers satisfy the composition law of the cyclic group G. In particular, we consider the representation R^n, and we consider a vector $v \in V^{(n)}$ in the subspace $V^{(n)}$ relative to this representation. Then the fundamental element of the group U_a is represented by an operator whose action on v is :

$$R^n(U_a)v = e^{i2\pi n/l}v, n = 1, ..., l$$

(the representation R^l is the trivial representation). Finally, we can use Burnside's theorem to assert that there are no other non-equivalent irreducible representations.

2. Determine the transformation law of the eigenfunctions of $\hat{H}$ under the transformations of the symmetry group G.
   We can separate the space of eigenfunctions of $\hat{H}$ into l subspaces $\mathcal{H}^{(n)}$, $n = 1, ..., l$ of dimension 1, relative to the l representations R^n. The eigenfunction $\psi_n(x) \in \mathcal{H}^{(n)}$ transforms according to the transformation law of the representation R^n, i.e. :

$$P_{U_a^n}\psi_n(x) = R^n(U_a)\psi_n(x) = e^{i2\pi n/l}\psi_n(x) = e^{ik_n a}\psi_n(x) = \psi_n(x+a),$$

   where $k_n = (2\pi/L)n$. Given this correspondence, it is more intuitive to use the wave vector k as an index for the subspaces instead of n.

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.
   We write the function $\psi_k(x)$ as :

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

   and using the transformation law of ψ_k. We find :

$$u_k(x)e^{ik(x+a)} = e^{ika}\psi_k(x) = \psi_k(x+a) = u_k(x+a)e^{ik(x+a)},$$

   So the functions u_k are periodic : $u_k(x+a) = u_k(x)$.

4. 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 : $\psi_k = \sum_{n=0}^{l-1} C_{k,n}\varphi_0(x-na)$. 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.

   4a. What is the Bloch wavefunction u_k assuming the tight-binding approximation ?

   (Questions 4a and 4b are non-examinable)

   As it was shown above, the Bloch theorem implies that the stationary states can be taken in the form $\psi_k(x) = u_k(x)e^{ikx}$. This property is a completely general result, which has its origin in group theory and in the symmetry properties of the system and, thus, it remains true

also in the tight-binding approximation. This implies that, also in the framework of the tight-binding approximation, the wave functions can be chosen in the form $u_k(x)\mathrm{e}^{ikx}$. At the same time, in tight binding, the stationary states can be taken in the form of linear superpositions $\sum_{p=0}^{l-1} C_{\gamma,p}\varphi_0(x-pa)$, where the index p runs over the l sites of the lattice. In this expression γ is an index specifying different solutions of the tight binding problem. In other words, we are considering solutions which are in the form of quantum superpositions of states localized near different atoms. We are thus approximating the wavefunctions as if they were living in an l-dimensional Hilbert space : instead of considering all possible functions we take only superposition of the l basis states $\varphi_0(x-pa)$. In this l-dimensional Hilbert space we can find l tight-binding states which are approximations to l stationary states of the full Schrödinger equation. The index γ labels these l distinct tight-binding superpositions.
Since we know that the functions can be written as $u_k(x)e^{ikx}$ we can match

$$u_k(x)e^{ikx} = \sum_{p=0}^{n-1} C_{\gamma,p}\varphi_0(x-pa) \ . \tag{21}$$

Since according to the Bloch theorem $u_k(x)$ is periodic, we have that

$$\sum_{p=0}^{n-1} C_{\gamma,p}e^{-ikx}\varphi_0(x-pa) = u_k(x) \tag{22}$$

must also be periodic with a period a (the lattice spacing).
Then we must have

$$\begin{aligned}
&\sum_p C_{\gamma,p}\mathrm{e}^{-ikx}\varphi_0(x-pa) = P_{U_a}\sum_p C_{\gamma,p}e^{-ikx}\varphi_0(x-pa)\\
&= \sum_p C_{\gamma,p}e^{-ik(x+a)}\varphi_0(x-(p-1)a)\\
&= \sum_p C_{\gamma,p+1}e^{-ik(x+a)}\varphi_0(x-pa) \ ,
\end{aligned} \tag{23}$$

where in the last step we shifted the dummy summation index p via the change of variables $p \to p+1$. The equation implies that

$$C_{\gamma,p+1}\mathrm{e}^{-ika} = C_{\gamma,p} \ , \tag{24}$$

and thus that

$$C_{\gamma,p} \propto e^{ipka} \ , \tag{25}$$

up to a proportionality constant.
This shows that the index γ, which labels different solutions, can be identified with the number k, which identifies different representations of the translation groups. For each k we have a different corresponding solution. Thus, in the following, we identify $\gamma = k$ to simplify the notation.
Introducing explicitly a normalization factor in Eq. (25), we can then write

$$C_{k,p} = \frac{1}{Z_k^{1/2}}e^{ipka} \ . \tag{26}$$

Then the tight-binding wavefunction with wavenumber k is

$$\psi_k(x) = \frac{1}{Z_k^{1/2}}\sum_p e^{ipka}\varphi_0(x-pa) \ , \tag{27}$$

and the corresponding Bloch wavefunction is

$$u_k(x) = \frac{1}{Z_k^{1/2}} \sum_p e^{ipka-ikx} \varphi_0(x-pa) = \frac{1}{Z_k^{1/2}} \sum_p e^{-ik(x-pa)} \varphi_0(x-pa) \ . \tag{28}$$

The fact that $u_k(x)$ is periodic can be seen from the fact that the terms in the sum depend only on $x-pa$. Thus, the translation $x \to x+a$, is cancelled by a shift $p \to p+1$ of the dummy index p, leading to a periodic result. In group theoretic language $u_k(x)$ transforms according to the trivial representation of the translation group (all translations are represented simply by the identity : the function $u_k(x)$ is invariant under translations). The wavefunction $\psi_k(x)$, by contrast, transforms according to a nontrivial representation of the group. The translation U_a is represented by the multiplication of a phase factor e^{ika}, and a translation of m steps, U_a^m is represented accordingly by e^{imka}.

To simplify the main derivation, we have slightly shortened the discussion of the effects of periodic boundary conditions. One possible way to represent the problem is to visualize it as if it was defined on a ring whose total circumference is L. This representation implements automatically that the coordinates x and $x+L$ are identified, as these correspond to the same point, after a complete turn around the circle. The problem on the circle, is then equivalent to the one-dimensional problem with periodic boundary conditions.

In this representation, the atoms are located at points whose polar coordinates are $(r_p = L/(2\pi), \theta_p = 2\pi p/l)$, $p = 0, ..., l-1$ and the continuous coordinate x corresponds to $L\theta/2\pi$, where θ is the polar angle. Writing the wavefunction as

$$\psi_k(x) = \frac{1}{Z_k^{1/2}} \sum_{p=0}^{l-1} e^{ipka} \varphi_0(x-pa) \ , \tag{29}$$

we can then verify, with a more explicit treatment of boundary conditions,

$$\begin{aligned} P_{U_a}\psi_k(x) = \psi_k(x+a) &= \frac{1}{Z_k^{1/2}} \sum_{p=0}^{l-1} e^{ipka} \varphi_0(x-(p-1)a) \\ &= \frac{1}{Z_k^{1/2}} \sum_{p=0}^{l-1} e^{ipka} \varphi_0(x-(p-1)a) = \frac{1}{Z_k^{1/2}} e^{ika} \sum_{p=-1}^{l-2} e^{ipka} \varphi_0(x-pa) \\ &= \frac{1}{Z_k^{1/2}} e^{ika} \sum_{p=0}^{l-2} e^{ipka} \varphi_0(x-pa) + \frac{1}{Z_k^{1/2}} e^{ika} e^{-ika} \varphi_0(x+a) \\ &= \frac{1}{Z_k^{1/2}} e^{ika} \sum_{p=0}^{l-2} e^{ipka} \varphi_0(x-pa) + \frac{1}{Z_k^{1/2}} e^{ika} e^{-ika} \varphi_0(x+a) \\ &= \frac{1}{Z_k^{1/2}} e^{ika} \sum_{p=0}^{l-2} e^{ipka} \varphi_0(x-pa) + \frac{1}{Z_k^{1/2}} e^{ika} e^{-ika} \varphi_0(x-L+a) \\ &= \frac{1}{Z_k^{1/2}} e^{ika} \sum_{p=0}^{l-1} e^{ipka} \varphi_0(x-pa) = e^{ika} \psi_k(x) \ . \end{aligned} \tag{30}$$

Here, it was used that x and $x-L$ are identified so that it can be assumed that $\varphi_0(x+a) = \varphi_0(x-L+a)$. It was also assumed that k takes one of the values $k = 2\pi n/L$, labeling the representations of the group, so that $e^{-ika} = e^{i(l-1)ka}$.

4b. Calculate the average energy of the state $\psi_k = u_k e^{ikx}$ in the tight-binding approximation.
To calculate the energy we need first to compute the normalization Z_k. This can be done imposing that the function ψ is normalized. The required normalization constant is :

$$Z_k = \sum_{p=0}^{l-1}\sum_{q=0}^{l-1}\int_0^L \mathrm{d}x\ \mathrm{e}^{i(p-q)ka}\varphi_0^*(x-qa)\varphi_0(x-pa)\ . \tag{31}$$

Physically, the orbitals located at *different* atoms have a small overlap, especially in a limit of "tight" binding, where the electrons are assumed to be strongly bound. Thus, the dominant term in the sum is $p = q$, which gives

$$Z_k = \sum_{p=0}^{l-1}\int_0^L \mathrm{d}x\ \varphi_0^*(x-pa)\varphi_0(x-pa) \simeq l\ . \tag{32}$$

We have assumed that the single-atom orbital are normalized to one and that the total size L of the system is much larger than the characteristic extension of a single atomic orbital. We then see that, keeping only the term, $p = q$, the normalization does not depend on k. In general, however, the corrections from terms $p \neq q$ introduce a correction which depends explicitly on k.
Having calculated the normalization factor, the average energy can be derived as :

$$\begin{aligned}
E_k &= \frac{1}{Z_k}\sum_{p=0}^{l-1}\sum_{q=0}^{l-1}\int_0^L dx\ e^{ik(p-q)a}\Big[\varphi_0^*(x-qa)\hat{H}\varphi_0(x-pa)\Big] \\
&= \frac{1}{Z_k}\sum_{p=0}^{l-1}\sum_{q=0}^{l-1}\int_0^L \mathrm{d}x\ e^{ik(p-q)a}\Big[\varphi_0^*(x-qa+pa)\hat{H}\varphi_0(x-pa+pa)\Big] \\
&= \frac{1}{Z_k}\sum_{p=0}^{l-1}\sum_{q=0}^{l-1}\int_0^L \mathrm{d}x\ e^{ik(p-q)a}\Big[\varphi_0^*(x+(p-q)a)\hat{H}\varphi_0(x)\Big]
\end{aligned} \tag{33}$$

where we used translational invariance and periodic boundary conditions (you can think of the representation of the problem on a ring).
The sum depends only on $p - q$. Making the change of variables $p \to p + q$ gives

$$\begin{aligned}
E_k &= \frac{l}{Z_k}\sum_{p=-q}^{l-1-q}\int_0^L \mathrm{d}x\ e^{ikpa}\Big[\varphi_0^*(x+pa)\hat{H}\varphi_0(x)\Big] \\
&= \frac{l}{Z_k}\sum_{p=0}^{l-1}\int_0^L \mathrm{d}x\ e^{ikpa}\Big[\varphi_0^*(x+pa)\hat{H}\varphi_0(x)\Big]\ ,
\end{aligned} \tag{34}$$

where we used again the boundary conditions. The energy receives contribution from "hopping" processes, in which the particle jumps between different potential wells.
As a remark, the tight-binding problem could also be defined on a line segment, assuming periodic boundary conditions for the wavefunction $\psi(x)$. In this case, the potential $V(x)$ should be defined by summing over infinitely many lattice sites $V(x) = \sum_{p=-\infty}^{\infty} u(x - pa)$, in order to have the translation-invariance property $V(x) = V(x + a)$.