1. Hermitean 2×2 Matrix

We will often encounter the problem of finding the eigenvalues and eigenvectors of a Hermitean 2×2 matrix. Show that the eigenvalues of the matrix

$$H = \begin{pmatrix} \epsilon & \Delta \\ \Delta^* & -\epsilon \end{pmatrix}$$

are $\pm W$ with $W = \sqrt{\epsilon^2 + |\Delta|^2}$ and that the normalized eigenvector for $-W$ is $(u, v)^T$ with

$$u = -\sqrt{\frac{W - \epsilon}{2W}} \qquad v = \frac{\Delta^*}{\sqrt{2W(W - \epsilon)}}$$

whereas the normalized eigenvector for $+W$ is $(u, v)^T$ with

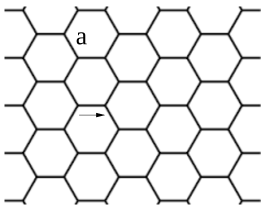
$$u = \sqrt{\frac{W + \epsilon}{2W}} \qquad v = \frac{\Delta^*}{\sqrt{2W(W + \epsilon)}}$$

Here 'normalized' means $|u|^2 + |v|^2 = 1$. Show that $|u|^2 - |v|^2 = \pm \frac{\epsilon}{W}$ and $uv^* = \frac{\Delta}{2W}$. Use the above to find the eigenvalues and eigenvectors of the more general matrix

$$H = \begin{pmatrix} \epsilon_1 & \Delta \\ \Delta^* & \epsilon_2 \end{pmatrix}.$$

2. Lattice Vectors and Brillouin Zone of the Honeycomb Lattice

For any crystal, the unit cell is defined as the smallest unit which produces the entire crystal when it is translated by all possible lattice vectors. For a two-dimensional lattice, the lattice vectors can be written as $\mathbf{R} = m \cdot \mathbf{R}_1 + n \cdot \mathbf{R}_2$ with integer m, n and the two basis vectors $\mathbf{R}_1$ and $\mathbf{R}_2$ (that means the two 'shortest' vectors which span the whole set of lattice vectors).
a) Find the unit cell and basis vectors of the honeycomb lattice:



The lattice is in the $x - y$ plane and consists of regular hexagons with an edge of a, one edge is parallel to the x-axis. Hint: First convince yourself that the vector indicated in the Figure is *not* a basis vector.
b) For a three-dimensional lattice the three reciprocal basis vectors $\mathbf{K}_i$ are defined by

$$\mathbf{K}_1 = \frac{2\pi}{V_c} \mathbf{R}_2 \times \mathbf{R}_3$$

plus two more equations obtained by cyclic permutation of the indices 1, 2, 3. Thereby $V_c = \mathbf{R}_1 \cdot (\mathbf{R}_2 \times \mathbf{R}_3)$ is the volume of the unit cell. Show that $\mathbf{K}_i \cdot \mathbf{R}_j = 2\pi\ \delta_{i,j}$.
For the two-dimensional honeycomb lattice we add the unit vector in z-direction, $\mathbf{e}_z$, as a 'nominal' third basis vector $\mathbf{R}_3$. Find the reciprocal basis vectors $\mathbf{K}_1$, $\mathbf{K}_2$ and $\mathbf{K}_3$. Show that whereas $\mathbf{K}_3$ points in z-direction, $\mathbf{K}_1$, $\mathbf{K}_2$ are in the $x - y$ plane. Sketch the reciprocal lattice which is formed by the vectors $\mathbf{K}_{m,n} = m \cdot \mathbf{K}_1 + n \cdot \mathbf{K}_2$ with integer m and n.
c) Determine the first Brillouin zone defined as the set of all $\mathbf{k}$ in the $x - y$ plane which obey

$$\mathbf{k} \cdot \mathbf{K}_{m,n} \leq \frac{1}{2}\,|\mathbf{K}_{m,n}|^2$$

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for all $\mathbf{K}_{m,n}$ with $m^2 + n^2 \neq 0$ (in other words: the set of all $\mathbf{k}$ whose distance from $(0, 0) = \mathbf{K}_{0,0}$ is $\leq$ their distance from any other $\mathbf{K}_{m,n}$). Show that the Brillouin zone has the form of a hexagon and find the coordinates of its corners. How would the results change if instead of $\mathbf{e}_z$ we had used the vector $\lambda\mathbf{e}_z$ with some real λ as the 'nominal' third basis vector?

3. Bloch theorem

The translation operator $T_{\boldsymbol{R}}$ is defined by its action on any function of the position:

$$T_{\boldsymbol{R}}\big(\phi(\boldsymbol{r})\big) = \phi(\boldsymbol{r} + \boldsymbol{R})$$

a) In one dimension choose $\phi(r) = r^2$ and sketch $T_{\boldsymbol{R}}\big(\phi(r)\big)$. Give a geometrical interpretation of TR.

b) Show that $T_{\boldsymbol{R_1}}T_{\boldsymbol{R_2}} = T_{\boldsymbol{R_1}+\boldsymbol{R_2}}$ and deduce that $\left[T_{\boldsymbol{R_1}}, T_{\boldsymbol{R_2}}\right] = 0$ for any $\boldsymbol{R_1}$ and $\boldsymbol{R_2}$. Show that $T_{n.\boldsymbol{R}} = (T_{\boldsymbol{R}})^n$.

c) Show that $T_{\boldsymbol{R}}$ commutes with the kinetic energy operator $T = \frac{-\hbar}{2m}\Delta$ (Hint: show that the commutator $\left[T_{\boldsymbol{R}}, \frac{\partial}{\partial x_i}\right]$ with i $\in \{1, 2, 3\}$ gives zero when acting on any function $\phi(\boldsymbol{r})$).

d) Consider the Hamiltonian $\mathcal{H} = T + V(\boldsymbol{r})$ and show that $\mathcal{H}$ commutes with $T_{\boldsymbol{R}}$ if the potential obeys $V(\boldsymbol{r}) = V(\boldsymbol{r} + \boldsymbol{R})$. Give a geometrical interpretation.

e) Show that if $\mathcal{H}$ commutes with $T_{\boldsymbol{R}}$, for any normalized eigenstate $\phi(r)$ of $\mathcal{H}$ (so $\mathcal{H}\phi = E\phi$ and $\int|\phi(r)|^2 dr = 1$), then $T_{\boldsymbol{R}}\phi(r)$ is also a normalized eigenstate of $\mathcal{H}$.

f) now consider a potential that is periodic on a crystal lattice defined by $\boldsymbol{R_{uvw}} = u\boldsymbol{R_1} + v\boldsymbol{R_2} + w\boldsymbol{R_3}$ (where u, v and w are integers). It can be shown that any nondegenerate eigenstates **of the** system $\phi(r)$ obeys $T_{\boldsymbol{R}_i}\big(\phi(\boldsymbol{r})\big) = exp(i\alpha_i)\phi(\boldsymbol{r})$. Define a reciprocal lattice vector $\boldsymbol{k} = \sum_{i=1}^{3}\frac{\alpha_i}{2\pi}\boldsymbol{K}_i$ (where the $\boldsymbol{K}_i$ are reciprocal lattice basis vectors - see problem 2). Express the phase factor α_{uvw} resulting from the application of $T_{\boldsymbol{R_{uvw}}}$ on $\phi(\boldsymbol{r})$ for an arbitrary vector $\boldsymbol{R_{uvw}}$ as function of $\boldsymbol{k}$. Show that for any reciprocal lattice vector $\boldsymbol{K}_{hkl}$, $\boldsymbol{k}$ and $\boldsymbol{k} + \boldsymbol{K}_{hkl}$ yield the same phase factor.

4. Periodic Boundary Conditions

We consider an infinite chain of points with coordinates $\mathbf{R}_n = (na, 0, 0)$, n integer, and the following functions defined on the set of these points: $f_k(n) = e^{ikna}$. Thereby k is a 'quantum number' of the function.

a) We now demand that $f_k(n)$ be periodic with period N: $f_k(n+N) = f_k(n)$ for any n. Find the values of k such that this condition is obeyed - from now we call these the 'allowed' k
(Hint: there are infinitely many of them...).

b) Show that if k is allowed, $k' = k + \frac{2l\pi}{a}$ (with l integer) is allowed as well and that $f_{k'}(n) = f_k(n)$ for any n - which means that either k or k' is redundant.

c) From now we assume that N is even. Find a 'minimum set' of nonredundant k, that means find a set of allowed k such that
i) no two k in the minimal set differ by $\frac{2l\pi}{a}$ with an integer $l \neq 0$
ii) any allowed k' not included in the minimal set can be written as $k' = k + \frac{2l\pi}{a}$ with some k in the minimal set
iii) The sum $\sum |k|$ taken over all k in the minimal set takes is as small as possible.
What is the number of k in the set?

d) Show that for any two allowed k and k'

$$\frac{1}{N} \sum_{n=1}^{N} f_k^*(n) f_{k'}(n) \quad = \quad \delta_{k,k'}.$$

(Hint: the expression on the left hand side is a geometric sum)

e) Now suppose we had demanded that f obeys the condition $f_k(n+N) = e^{i\Theta}\, f_k(n)$ for any n with $\Theta \in [0, 2\pi]$ - how would the results have changed?

f) Now we generalize the above to a three dimensional lattice. Consider a lattice of points with coordinates $\mathbf{R}_{l,m,n} = l\mathbf{R}_1 + m\mathbf{R}_2 + n\mathbf{R}_3$, where $\mathbf{R}_i$ are the three lattice vectors (see Problem 2). Our functions now are $f_{\mathbf{k}}(l,m,n) = e^{i\mathbf{k}\cdot\mathbf{R}_{l,m,n}}$ and we demand that the $f_{\mathbf{k}}$ are 'periodic in three directions' $f_{\mathbf{k}}(l+M,m,n) = f_{\mathbf{k}}(l,m+M,n) = f_{\mathbf{k}}(l,m,n+M) = f_{\mathbf{k}}(l,m,n)$, with some integer M. Find the allowed $\mathbf{k}$ (hint: check out the definition of a reciprocal lattice vector in problem 2) and find again a 'minimal set' of allowed $\mathbf{k}$. What is the number of $\mathbf{k}$ in the minimal set?