ATOMIC PHYSICS

- A Quick Guide -

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June 15, 2021

Preface

Greetings,

While I have spent most of my undergraduate years in Professor Charles Conover's lab at Colby College working on cold atom experiments, I never had *formal* training in atomic, molecular, and optical physics. The closest to formal training I have for AMO physics is a standard quantum mechanics course I took in the fall of my junior year. Most of the intuition I have for atomic physics, I learned from my discussions with Professor Conover or read from books and articles here and there. This article is my attempt at *formally* teaching myself atomic physics.

This article is basically my version of an "atomic physics dictionary," which should keep growing as I go along in my education and research at MIT. As a result of this, there is no good way for me to organize the topics in here but by alphabetical order (hence "dictionary"). I don't know how well I'll be able to curate this article, but we'll see.

In any case, good luck and, most importantly, enjoy!

A

B

Bloch's Theorem and Bloch States

Consider a periodic potential $V(\mathbf{r})$ associated with a lattice whose primitive lattice translation vectors are given by

$$\mathbf{T} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3,$$

where n_i are integers and $\mathbf{a_i}$ are the three noncoplanar vectors ($\mathbf{T}$ is basically vectors which translates from one vertex in the lattice to another arbitrary one). Since V is periodic, we have

$$V(\mathbf{T} + \mathbf{r}) = V(\mathbf{r}).$$

In Fourier components,

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}$$

where $\mathbf{G}$ are a set of vectors and $V_{\mathbf{G}}$ are Fourier coefficients. By the periodicity of V, we have

$$e^{i\mathbf{G}\cdot\mathbf{T}} = 1 \implies \mathbf{G}\cdot\mathbf{T} = 2\rho\pi, \quad \rho \in \mathbb{Z}.$$

The only way to define $\mathbf{G}$ such that the above equation makes sense is:

$$\mathbf{G} = m_1\mathbf{A}_1 + m_2\mathbf{A}_2 + m_3\mathbf{A}_3$$

where m_j are integers and $\mathbf{A}_j$ are three noncoplanar vectors defined by

$$\mathbf{a}_j \cdot \mathbf{A}_l = 2\pi\delta_{jl}$$

This shows the existence of an r-lattice implies that of a k-lattice, and we call $\mathbf{G}$ the reciprocal lattice.

What set of functions describes the motion of electrons in such a potential? Since we want to reflect the translation symmetry of the lattice, we may impose the *Born-von Karman periodic boundary condition* on the plane wave

$$\phi(\mathbf{r}) = e^{i(\mathbf{k}\cdot\mathbf{r} - \omega t)}$$

to get

$$\phi(\mathbf{r} + N_j \mathbf{a_j}) = \phi(\mathbf{r})$$

where $j = 1, 2, 3$ and $N = N_1 N_2 N_3$ is the number of primitive unit cells in the crystal; N_j is the number of unit cells in the jth direction. From here, we have that

$$e^{iN_j \mathbf{k}\cdot\mathbf{a}_j} = 1.$$

Following a similar argument as before, we find that the only allowed $\mathbf{k}$ vectors are of the form

$$\mathbf{k} = \sum_{j=1}^{3} \frac{m_j}{N_j} \mathbf{A}_j$$

Now, consider a Schrödinger equation with potential $V(\mathbf{r})$:

$$\widehat{H}\psi = \left[-\frac{\hbar^2 \nabla^2}{2m} + V(\mathbf{r}) \right] \psi = E\psi.$$

In Fourier components, we again have

$$V(\mathbf{r}) = \sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}}.$$

Let us set the background potential to zero, i.e., $V_0 \equiv 0$. Next, let us write the solution $\phi(\mathbf{r})$ as a combination of plane waves obeying the Born-von Karman PBC:

$$\psi(\mathbf{r}) = \sum_{\mathbf{k}} C_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}},$$

so that $\phi(\mathbf{r})$ also satisfies the Born-von Karman PBC. Plugging this into the SE, we find

$$\sum_{\mathbf{k}} \frac{\hbar^2 k^2}{2m} C_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} + \underbrace{\left[\sum_{\mathbf{G}} V_{\mathbf{G}} e^{i\mathbf{G}\cdot\mathbf{r}} \right] \left[\sum_{\mathbf{k}} C_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}} \right]}_{V(\mathbf{r}\psi)} = E \sum_{\mathbf{k}} C_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}}$$

where we can re-write:

$$V(\mathbf{r})\psi = \sum_{\mathbf{G},\mathbf{k}} V_{\mathbf{G}} C_{\mathbf{k}} e^{i(\mathbf{G}+\mathbf{k})\cdot\mathbf{r}} = \sum_{\mathbf{G},\mathbf{k}} V_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}} e^{i\mathbf{k}\cdot\mathbf{r}}.$$

With this, we can factor out $e^{i\mathbf{k}\cdot\mathbf{r}}$ in each term of the SE and use the fact that the plane waves form an orthogonal basis, we find

$$\left(\frac{\hbar^2 k^2}{2m} - E \right) C_{\mathbf{k}} + \sum_{\mathbf{G}} V_{\mathbf{G}} C_{\mathbf{k}-\mathbf{G}} = 0.$$

Let us write $\mathbf{k} = \mathbf{q} - \mathbf{G}'$ and let $\mathbf{G}'' = \mathbf{G}' + \mathbf{G}$, where $\mathbf{q}$ lies in the first Brillouin zone. With this change of variables, we have the result

$$\left(\frac{\hbar^2 (\mathbf{q} - \mathbf{G}')^2}{2m} - E \right) C_{\mathbf{q}-\mathbf{G}'} + \sum_{\mathbf{G}''} V_{\mathbf{G}''-\mathbf{G}'} C_{\mathbf{q}-\mathbf{G}''} = 0.$$

Now, we're ready for the statement of the **Bloch's Theorem**. The result above involves coefficients $C_{\mathbf{k}}$ in which $\mathbf{k} = \mathbf{q} - \mathbf{G}$, where $\mathbf{G}$ are general reciprocal lattice vectors. This means that if we fix $\mathbf{q}$, then the only $C_{\mathbf{k}}$ that feature are of the form $C_{\mathbf{q}-\mathbf{G}}$. In other words, for each $\mathbf{q}$, there is a wavefunction $\psi_{\mathbf{q}}(r)$ that takes the form

$$\psi_{\mathbf{q}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{\mathbf{q}-\mathbf{G}} e^{i(\mathbf{q}-\mathbf{G})\cdot\mathbf{r}},$$

where we have substituted $\mathbf{k} = \mathbf{q} - \mathbf{G}$. Factoring out $e^{i\mathbf{q}\cdot\mathbf{r}}$, we find

$$\boxed{\psi_{\mathbf{q}}(\mathbf{r}) = e^{i\mathbf{q}\cdot\mathbf{r}} \sum_{\mathbf{G}} C_{\mathbf{q}-\mathbf{G}} e^{-i\mathbf{G}\cdot\mathbf{r}} \equiv e^{i\mathbf{q}\cdot\mathbf{r}} u_{j,\mathbf{q}}}$$

So, the solution is a plane wave with wave vector within the first Brillouin zone TIMES a function with the periodicity of the lattice. Functions of this form are known as **Bloch functions** or **Bloch states**. They serve as a suitable basis for the wave functions or states of electrons in crystalline solids.

Bloch's Theorem is as follows: *The eigenstates ψ of a one-electron Hamiltonian defined above for all Bravais lattice translation vectors* $\mathbf{T}$ *can be chosen to be a plane wave times a function with the periodicity of the Bravais lattice.* We note two things:

- This is true for any particle propagating in a lattice
- The theorem makes no assumption about the *strength/depth* of the potential.

Notes: The terminologies in blue can be found in [1] or Wikipedia. The concepts are simple enough, so I won't include their definitions here.

C

D

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E

F

Feshbach Resonance

G

H

I

K

L

M

N

O

P

Q

Quantum Harmonic Oscillator

R

Raman side-band cooling

Recoil temperature

S

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T

U

V

W

X

Y

Z

Bibliography

[1] C. Kittel, P. McEuen, and P. McEuen, *Introduction to solid state physics*, vol. 8. Wiley New York, 1996.