PHY215-06: Quantum Mechanics

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1 Bohr's Atomic Model and de Broglie's Matter Waves

1.1 Bohr's Atomic Model (1913)

Niels Bohr proposed his atomic model to explain hydrogen's stability and discrete emission spectrum using three postulates:

- **Quantization of Angular Momentum**

  $$L = mvr = n\hbar \quad (n = 1, 2, 3, \dots),$$

  where L is angular momentum, m is electron mass, v is orbital velocity, r is orbital radius, n is the principal quantum number, and $\hbar = h/(2\pi)$.

  - This ad hoc assumption enforced discrete orbits to avoid classical radiative collapse.

- **Stationary Orbits and No Radiation** - Electrons in quantized orbits do not radiate energy despite acceleration (contradicts classical electromagnetism). - Stability arises from the quantum condition $L = n\hbar$.

- **Radiation During Transitions**

  $$E_{\text{photon}} = \Delta E_{\text{atom}} = \frac{hc}{\lambda} = E_{n_2} - E_{n_1}.$$

  - Explains hydrogen's spectral lines (e.g., Balmer series).

1.1.1 Predictions

Consider a scenario where a single electron orbits a nucleus containing Z protons.

- **Orbital Radius**

$$r_n = \frac{4\pi\epsilon_0\hbar^2}{me^2 Z}n^2 = \frac{n^2}{Z}a_0,$$

where the Bohr radius of Hydrogen atom (with atomic number $Z = 1$) for $n = 1$ is $a_0 = 0.529\,\text{Å} = 0.529 \times 10^{-10}\ m$.

- **Energy Levels**

$$E_n = -\frac{me^4 Z^2}{2\hbar^2 n^2 (4\pi\epsilon_0)^2} = -\frac{Z^2}{n^2}E_0,$$

where the ionization energy of the Hydrogen atom is $E_n = 13.6\,\text{eV}$.

- **Speed of orbital electron**

$$v_n = \frac{e^2 Z}{4\pi\epsilon_0\hbar}\frac{1}{n} = \frac{Z}{n}\alpha c \equiv \frac{Z}{n}v_0,$$

where the fine structure constant is

$$\alpha \equiv \frac{e^2}{4\pi\epsilon_0\hbar c} \simeq \frac{1}{137}.$$

Note that the orbital angular momentum $L_n = mr_n v_n = n\hbar$, so that for $n = 1$ and $Z = 1$,

$$v_0 = \alpha c, \qquad a_0 = \frac{\hbar}{mv_0} = \frac{\hbar}{m\alpha c}, \qquad E_0 = \frac{1}{2}m(\alpha c)^2.$$

- An example of Lithium iron

Lithium (^{3}Li) has an atomic number of 3. Hence, its nucleus has 3 protons. Lithium-7 has an atomic mass of 7. Given that its atomic number is 3, there are 7 - 3 = 4 neutrons in its nucleus. Since atoms are charge neutral, the ^{3}Li atom has 3 electrons. Thus, the Lithium (^{3}Li^{++}) iron has one electron.

1.1.2 Fine structure constant

The fine-structure constant (α) is a dimensionless fundamental constant that characterizes the strength of electromagnetic interactions. Its expression in terms of Planck's constant (h) and the speed of light (c) is:

$$\alpha = \frac{e^2}{4\pi\varepsilon_0} \cdot \frac{1}{\hbar c},$$

where:
- e is the elementary charge,
- ε_0 is the vacuum permittivity,
- $\hbar = \frac{h}{2\pi}$ is the reduced Planck constant.
- Its current Value:

The latest CODATA (2018) recommended value of α is:

$$\alpha \approx 0.0072973525693 \quad (\text{approximately } \frac{1}{137.035999206}).$$

Running coupling constant

The fine-structure constant depends on energy in the context of quantum field theory. This phenomenon is known as “running coupling constants” and arises due to quantum corrections (virtual particle-antiparticle pairs) modifying the effective strength of electromagnetic interactions at different energy scales.

In quantum electrodynamics (QED), the effective value of α increases slightly with energy. This is because higher-energy interactions probe closer to the bare electron charge, where the screening effect of virtual electron-positron pairs is reduced.

$\alpha \sim \frac{1}{137}$ at low energy scale (about zero), and it runs to about $\frac{1}{128}$ at high energy scale (about 100 GeV).

Note that in terms of the absolute temperature Kelvin (K), $1\,\mathrm{eV} \sim 10^4 K$, so $1\,\mathrm{GeV} \sim 10^{13} K$.

1.2 Comparison with de Broglie’s Theory

- **Classical vs. Wave-Based** - Bohr retained classical mechanics with quantum constraints. - de Broglie replaced orbits with matter waves and standing-wave conditions.

- **Assumptions** - Bohr’s $L = n\hbar$ lacked justification until de Broglie linked it to electron wavelengths.

- **Success/Limitations** - Explained hydrogen spectrum but failed for multi-electron atoms. - de Broglie provided a unifying wave-particle duality framework.

1.3 de Broglie's Matter Wave Hypothesis

Louis de Broglie's theory provided a wave-based explanation for Bohr's stationary orbits:

1. **Matter Wave Hypothesis**

$$\lambda = \frac{h}{p} \quad \text{(de Broglie wavelength)},$$

where $p = mv$ is electron momentum.

2. **Stationary Orbits as Standing Waves**

$$2\pi r = n\lambda \quad (n = 1, 2, 3, \dots).$$

3. **Derivation of Bohr's Quantization Rule**

$$2\pi r = n \cdot \frac{h}{mv} \quad \Rightarrow \quad mvr = \frac{nh}{2\pi}.$$

Since $L = mvr$:

$$L = \frac{nh}{2\pi} = n\hbar.$$

4. **Physical Interpretation** - Standing waves require integer multiples of λ, preventing destructive interference. - Resolves classical paradox of non-radiating electrons.

1.3.1 Key Contributions

- Unified particle and wave descriptions. - Provided theoretical justification for Bohr's quantization. - Laid groundwork for wave mechanics.

2 Phase velocity and group velocity

2.1 Wave packet

According to the superposition principle, the combination of two plane waves can illustrate the distinction between phase velocity and group velocity. Below is the detailed derivation:

2.1.1 The Superposition of Two Plane Waves

Consider two plane waves with wave vectors k_1 and k_2, angular frequencies ω_1 and ω_2, and equal amplitude A. Their superposition yields:

$$\psi(x,t) = Ae^{i(k_1x-\omega_1t)} + Ae^{i(k_2x-\omega_2t)}. \tag{1}$$

2.1.2 Simplification via Trigonometric Identities

Assume $k_1 \approx k_2$ and $\omega_1 \approx \omega_2$. Define average and difference quantities:

$$k_{\text{avg}} = \frac{k_1+k_2}{2}, \qquad \Delta k = \frac{k_1-k_2}{2}, \tag{2}$$

$$\omega_{\text{avg}} = \frac{\omega_1+\omega_2}{2}, \qquad \Delta\omega = \frac{\omega_1-\omega_2}{2}. \tag{3}$$

Rewrite the wavefunction as:

$$\psi(x,t) = Ae^{i(k_{\text{avg}}x-\omega_{\text{avg}}t)}\left[e^{i(\Delta kx-\Delta\omega t)} + e^{-i(\Delta kx-\Delta\omega t)}\right]. \tag{4}$$

Using $e^{i\theta} + e^{-i\theta} = 2\cos\theta$, we obtain:

$$\psi(x,t) = 2A\cos\left(\Delta kx - \Delta\omega t\right) \cdot e^{i(k_{\text{avg}}x - \omega_{\text{avg}}t)}. \tag{5}$$

2.1.3 Separating Envelope and Carrier

The superposed wave consists of:

- **Carrier Wave**: The high - frequency oscillation $e^{i(k_{\text{avg}}x - \omega_{\text{avg}}t)}$, with phase velocity:
  $$v_p = \frac{\omega_{\text{avg}}}{k_{\text{avg}}}. \tag{6}$$
- **Envelope**: The low - frequency modulation $2A\cos\left(\Delta kx - \Delta\omega t\right)$, with group velocity:
  $$v_g = \frac{\Delta\omega}{\Delta k}. \tag{7}$$

2.1.4 Physical Interpretation

- **Phase Velocity** v_p: The speed of individual wave crests/troughs, describing phase propagation.
- **Group Velocity** v_g: The speed of the wave packet (energy/information), defined by the derivative:
  $$v_g = \frac{d\omega}{dk} \quad \text{(in the limit } \Delta k \to 0\text{)}. \tag{8}$$

2.1.5 Examples: Non - Dispersive vs. Dispersive Media

- **Non-Dispersive Media (e.g., electromagnetic waves in vacuum)**: $\omega = ck$, so $v_p = v_g = c$.
- **Dispersive Media (e.g., light in glass)**: $\omega \neq ck$, leading to $v_p \neq v_g$.

2.1.6 Conclusion

By superposing two plane waves, we visually demonstrate the separation between phase velocity (carrier speed) and group velocity (envelope speed). In dispersive media, these velocities differ; in non - dispersive media, they coincide.

2.2 The comparison of electron and photon

Here's a comparison table of phase velocity and group velocity for non-relativistic and relativistic electrons (matter waves) and photons, based on their dispersion relations:

Property	Electron		Photon
	Non-Rel.	Rel.	
Dispersion Relation	$\omega = \frac{\hbar k^2}{2m}$	$\omega = \sqrt{c^2k^2 + \left(\frac{mc^2}{\hbar}\right)^2}$	$\omega = ck$
Phase Vel. ($v_p = \frac{\omega}{k}$)	$v_p = \frac{\hbar k}{2m} = \frac{v}{2}$	$v_p = c\sqrt{1 + \left(\frac{mc}{\hbar k}\right)^2}$	$v_p = c$
Group Vel. ($v_g = \frac{d\omega}{dk}$)	$v_g = \frac{\hbar k}{m} = v$	$v_g = \frac{c^2k}{\omega} = \frac{c^2}{v_p}$	$v_g = c$
Key points	$v_p < v_g$	$v_p > c$, $v_g < c$	$v_p = v_g = c$

Key Notes:

1. For non - relativistic electrons:
- Energy $E = \frac{p^2}{2m}$, with $p = \hbar k$ and $E = \hbar\omega$. Note that $k = \frac{2\pi}{\lambda}$ and $\omega = 2\pi f$.
- Phase velocity $v_p = \frac{v}{2}$
- Group velocity $v_g = v$ (matches classical velocity)
2. For relativistic electrons:
- Energy $E = \sqrt{(pc)^2 + (mc^2)^2}$, with $p = \hbar k$ and $E = \hbar\omega$.
- Phase velocity $v_p > c$, but group velocity $v_g < c$
- As $k \to \infty$, $v_g \to c$
3. Photons in vacuum:
- Energy $E = pc$, with $p = \hbar k$ and $E = \hbar\omega$.
- Perfect linear dispersion ($\omega \propto k$)
- No spreading of wave packets (non-dispersive)
4. Causality is preserved because energy/momentum propagate at v_g, not v_p

3 Gaussian Wave Packet Representation

A Gaussian wave packet can be expressed as a superposition of plane waves through a Fourier transform. Here's the mathematical formulation:

3.1 Gaussian Wave Packet in Position Space

A Gaussian wave packet centered at position x_0 with width σ is:

$$\psi(x) = \left(\frac{1}{\pi\sigma^2}\right)^{1/4} e^{-\frac{(x-x_0)^2}{4\sigma^2}} e^{ip_0x/\hbar}.$$

- p_0: Central momentum of the wave packet. - The normalization factor $\left(\frac{1}{\pi\sigma^2}\right)^{1/4}$ ensures $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$.

3.2 Superposition of Plane Waves

To represent $\psi(x)$ as a superposition of plane waves $e^{ipx/\hbar}$, we use the Fourier transform:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \phi(p)\, e^{ipx/\hbar}\, dp,$$

where $\phi(p)$ is the momentum-space wave function. For the Gaussian wave packet, $\phi(p)$ is also Gaussian:

$$\phi(p) = \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{1/4} e^{-\frac{\sigma^2(p-p_0)^2}{\hbar^2}} e^{-ipx_0/\hbar}.$$

3.2.1 Key Relationships

1. **Widths in Position and Momentum Spaces**:

$$\begin{aligned} \text{Position uncertainty:} \qquad & \Delta x = \sigma, \\ \text{Momentum uncertainty:} \qquad & \Delta p = \frac{\hbar}{2\sigma}, \\ \text{Uncertainty relation:} \qquad & \Delta x \Delta p = \frac{\hbar}{2}. \end{aligned}$$

2. **Plane Wave Superposition**: The wave packet $\psi(x)$ is built by summing plane waves $e^{ipx/\hbar}$ with weights $\phi(p)$, encoding probability amplitudes for each momentum p.

3.2.2 Final Expression

Substituting $\phi(p)$ into the Fourier integral:

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{2\sigma^2}{\pi\hbar^2}\right)^{1/4} \int_{-\infty}^{\infty} e^{-\frac{\sigma^2(p-p_0)^2}{\hbar^2}} e^{-ipx_0/\hbar} e^{ipx/\hbar} \, dp.$$

This simplifies to the original Gaussian wave packet in position space, confirming equivalence.