

Quantum Mechanics: Discretization of Energy and Wave-Particle Duality

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1 Introduction

Classical physics (derived from the ideas of Newton, Hamilton, Lagrange and other early physicists) encountered several experimental observations that it could not fully resolve within its formalisms and constructs. This occurred during the turn of the 20th century. Here we briefly discuss the canonical historical experiments that led to the understanding of the discrete nature of energies of matter at the atomic level, as well as the wave-particle duality of matter on the same lengthscales.

2 Blackbody Radiation and the UV Catastrophe

We know intuitively that objects at a particular temperature radiate electromagnetic (em) energy; we emphasize that the energy is not just in the visible range of the em spectrum, but spans, in theory, the entire range. Consider a space heater, glowing embers of a fire, glowing charcoal embers, an incandescent light bulb, a kitchen oven, etc. In each case, we know intuitively that there is associated some radiation of energy corresponding to the temperature of the body (we can feel the heat around each of the bodies mentioned). An idealization of these types of systems is the black body emitter. The black body emits radiation that is in thermal equilibrium at the temperature of the body.

We can now speak of the **spectral density** of the body. The spectral density is the *energy stored in the em field of the blackbody emitter at frequency ν per unit volume and unit frequency*.

$$\rho(\nu, T) = \frac{8 \pi \nu^2}{c^3} \langle E_{oscillator} \rangle$$

The total energy per unit volume in a small range of frequencies $d\nu$ is

$$\rho(\nu, T) d\nu = \frac{8 \pi \nu^2}{c^3} \langle E_{oscillator} \rangle d\nu$$

The origin of the black body emitter's energy is taken to be from the **oscillatory** behavior of the atoms (nuclei and electrons) making up the body; the approximation is simple and loosely approximates a solid material, where the combination of positive nucleus and negative electronic clouds of atoms represent oscillating electric dipoles (in a classical sense).

Classical physics treats the oscillator energy $E_{oscillator}$ as:

$$\langle E_{oscillator} \rangle = k_B T$$

Use of the latter expression leads to an expression for the amount of energy per unit volume in the frequency range from ν to $\nu + d\nu$ as:

$$\rho(\nu, T) d\nu = \frac{8 \pi \nu^2 k_B T}{c^3} d\nu$$

- *Classical theory predicts a quadratic dependence of energy on frequency.*
- The amount of energy given off by a classical black-body (taken to be the area under the curve) is infinite, in stark contrast to experimentally determined curves which show that the distribution is peaked about some average frequency, and then drops off at higher and lower frequencies.
- Classical physics treats low frequency behavior correctly, but does not capture high frequency behavior (UV catastrophe).

Max Planck hypothesized that the relation for oscillatory energy was incorrect. The error originated in the description of the energy of a single oscillator. He suggested the following relation:

$$E = n h \nu$$

where h is Planck's constant (determined independently at a later time) and n is some integer. This is another way of saying that the energy of an oscillator of frequency ν is discretized (or quantized) and can take on only integer values (dictated by the n in the relation). Thus, Planck foresaw the need for a discrete (versus continuous) description of energy in the quantum context.

With this in mind, the oscillatory energy becomes:

$$\langle E_{osc} \rangle = \frac{h \nu}{e^{h\nu/kT} - 1}$$

The spectral density Planck obtained using this expression is:

$$\rho(\nu, T) d\nu = \frac{8 \pi h \nu^2}{c^3} \frac{1}{e^{h\nu/kT} - 1} d\nu$$

The above relation matches experiment very well, and Planck was able to use this expression to fit h to experimental data.

The breakthrough Planck contributed was the idea of **discretization of energy**.

3 Photoelectric Effect

The experiment:

- shine light (em radiation) on a metal plate (i.e., copper) placed in vacuum (evacuated chamber).
- incident light absorbed by atoms and electrons excited to higher energy levels.
- provide sufficient light energy to eject electrons from atoms and the metal
- from classical conservation of energy arguments, the kinetic energy of the emitted electron is equal to the incident light energy minus the energy required for ejection:

$$KE = E_{incident} - E_{ejection}$$

For the above experiment describing the photoelectric effect, the following predictions are made by classical theory; along with the predictions are given the experimental outcomes for contrast.

- **Classical:** Electrons are emitted for all frequencies provided the light is sufficiently *intense*
Experiment: No electrons are emitted unless the frequency of incoming light is a threshold value; this is independent of the intensity of the incoming light
- **Classical:** The kinetic energy per electron increases with the light intensity
Experiment: The kinetic energy of an electron depends on the frequency in a linear manner

- **Classical:** Light is incident over the entire surface as a **plane wave**. Any one atom receives a small portion of the total energy
Experiment: Electrons are emitted even at such low intensities that all the light absorbed by the plate is barely enough to eject a single electron based on energy conservation considerations.

As with black body radiation, classical theory was not consistent with experimental observations. To explain the photo electric effect, Einstein proposed that the **energy of light was proportional to its frequency:**

$$E = \beta \nu$$

Classical physics gave no relation between the energy of a light wave and its frequency; this idea was a radical departure.

The energy of an ejected electron is now given by:

$$E_e = \beta \nu - \phi$$

where ϕ is the **work function** of the metal; this is the binding energy of the electron in the solid, or the ionization energy of the atom.

The linear relation between electron energy and frequency of incident light allowed β to be determined. Its value turns out to be Planck's constant, h . Thus

$$E = h \nu$$

A final note. That the photoelectric effect allows for electron ejection even at such low intensities that the total energy just slightly exceeds the work function of the metal. This suggests that the energy reaching an atom whose electron is ejected is **spatially localized**; this idea led to the term of a **photon**, a spatially localized packet of energy. In this sense, light was now given a **particle-like** characteristic; it was spatially localized like a particle as well as more diffuse according to the well-accepted classical description as wave. This is the wave-particle duality of quantum mechanics.

4 Diffraction of Electrons; Wave-Particle Duality; Superposition; Measurements and Collapse

Having encountered the idea of wave-particle duality, we present a result formalized by Louis de Broglie relating the wavelength of a particle to its momentum:

$$\lambda = \frac{h}{p}$$

where p is the particle momentum given by $p = m v$.

This relation was verified by Davisson and Germer in their experiment on electron diffraction by NiO in 1927. Considering particles as wave-like required a formulation of their dynamics in terms of a wave equation (analogous to the classical dynamics given by Newtonian mechanics and Newton's laws). This was accomplished by Schroedinger.

We next consider electron diffraction in the following discussion.