Quantum Mechanics-I Lecture Notes[1]

Part- I Rise of Quantum Mechanics

Planned for A Course Be at IIT Bhubaneswar

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Lecture 1

Inadequacy of Classical Theories

There were several experiments which pointed to inadequacy of the classical thoeries such as mechanics,electromagnetic theory of light, and statistical mechanics. Here we list some of the important experimental facts which had no explanation within the classical theories.

1. Black Body radiation
2. Photoelectric effect
3. Atomic spectra
4. Frank Hertz experiment
5. Compton effect
6. Stern Gerlach Experiment
7. Zeeman splitting of spectral lines in magnetic field
8. Stark effect
9. Wave nature of electrons
10. Alpha decay
11. Beta decay
12. Specific heat of solids and gases

While efforts to explain some of the above experiments played crucial role in the development of quantum theory, Some other experiments provided crucial support for proposals during 1900-1925, before quantum mechanics was born in 1926. Still an explanation of some others had to wait for a fully developed quantum mechanics.

Lecture 2

Rise of quantum theory

1. **Planck's theory Black body radiation (1900)**
   In order to explain the black body radiation Planck introduced assumption that the radiation is not emitted continuously but in form of packets of energy.

2. **Einstein's paper on photoelectric effect (1905)**
   Einstein's explanation of photoelectric effect brought in the particle nature back and led to acceptance of dual nature of radiation. A crucial assumption was that energy of a photon of frequency is $E = h\nu$ and that absorption of light can takes place only by absorbing one or more photons, energy from light is not absorbed continuously as was assumed in the classical electromagnetic theory.

3. **Bohr's theory of H atom spectra (1913), Franck Hertz experiment (1914)**
   Bohr assumed that all orbits are not allowed and an electron does not radiate in certain states, called stationary states. To find the allowed orbits and corresponding energies, Bohr assumed that the angular momentum of the electron can only take values equal to integral multiples of Planck's constant $\hbar$. This rule was later reformulated as the Bohr Sommerfeld quantisation rule.

   Discrete nature of atomic energy levels was confirmed by the Franck Hertz experiment.

4. **Wilson Sommerfeld Quantisation (1916)** The quantisation rule

   $$\oint pdq = nh$$

   generalized the qunatization of angular momentum used by Bohr's and was found useful for wider applications, one example being relativistic corrections to hydrogen atom levels. Notable failure of this rule was the spectrum of He atom.

5. **Zeeman effect (1896-1916)**
   Normal Zeeman effect observed (1896), in some atoms, was explained by Lorentz

(1897) using classical electromagnetic theory. It came to be called normal Zeeman effect.After Bohr model was published, Sommerfeld and Debye, independently, gave a explanation of the observed pattern within older quantum theory (1916) before quantum mechanics was born. It required the assumption that the component of angular momentum along the magnetic field is quantized.

The Zeeman pattern in most atoms is very complex and an explanation had to wait for introduction of spin of electron.

6. **Compton Scattering (1923)** The experimental results on scattering of X-rays by atoms firmly established, beyond any doubt, the corpuscular nature of radiation. In addition to establishing the particle picture for light, the energy momentum relation $E = pc$, a prediction of special relativity was beautifully confirmed by Compton scattering data.

7. **Heisenberg's Matrix mechanics(1925)** While trying to understand intensities of spectral lines of hydrogen spectrum, Heisenberg laid foundations of matrix mechanics. During this investigation he sought to reformulate Sommerfeld quantisation condition

$$\oint pdq = nh$$

and arrived at

$$h = 4\pi nm \sum_{\alpha=0}^{\infty} \big\{ |a(n, n+\alpha|^2 \omega(n+\alpha) - |a(n, n-\alpha)|^2 \omega(n, n-\alpha) \big\}. \tag{2.1}$$

In this work Heisenberg assumed that the probabilities of transition from n to $n-\alpha$ was proportional to $|a(n, n-\alpha)|^2$. This paper was written in middle of July 1925 and was sent to Max Born. Max Born wrote Heisenberg's equation in the form

$$\sum_k \big[p(n,k)q(k,n) - q(n,k)p(k,nn) = \frac{h}{2\pi i} \tag{2.2}$$

and realised that the relations was diagonal element of the matrix form of quantum condition

$$pq - qp = \frac{h}{2\pi i} I. \tag{2.3}$$

To learn more about Eq.(2.1) *refer to Heisenberg's original paper.* Matrix mechanics was eventually completed by Heisenberg, Born and Jordan by October 1925 and was applied to quantisation of electromagnetic field.

8. **Canonical quantisation(1925)** Dirac brought in the correspondence of matrix commutator in quantum theory with Poisson brackets in classical theory. Fowler had asked Dirac to give his comments on the manuscript of Heisenberg's paper.

Dirac went on to develop full abstract machinery of quantum mechanics as we know today. Pauli, who had been initially critical of formal matrix approach, solved the hydorgen atom problem within the matrix mechanics.

9. **Matter waves(1924)** The idea of associating waves with material particles was introduced by de Broglie. This was confirmed by beautiful experiment of Davisson and Germer on electron diffraction (1927). The data of 1921 experiments was already pointing towards effects of diffraction.

10. **Bose Einstein Statistics (1924)** Bose's derivation of black body radiation opened the doors for treatment of systems of identical particles and quantum statistics.

11. **Introduction of spin (1925)**
    Goudsmith and Uhlenbeck's idea to introduce spin was crucial to understanding Stern Gerlach experiment, anomalous Zeeman effect and the fine structure of atomic spectra. Heisenberg and Jordan completed the solution to the problem of anomalous Zeeman effect within matrix mechanics.

12. **Pauli exclusion principle (1925) and periodic Table**

13. **Quantisation as an eigenvalue problem (1926)** Schrödinger as an attempt developed wave mechanics as an alternative to the Matrix mechanics of Born Jordan Dirac and Heisenberg. He proposed quantisation as an eigenvalue problem and solved the Hydrogen atom problem. Schrodinger went on to prove equivalence of wave mechanics with matrix mechanics, discovered independently by Eckart (1926).

14. **Probability in quantum mechanics (1926)** The probabilistic nature already appeared in Heisenberg's work. Working on anomalous Zeeman effect he assumed that the intensities were proportional to absolute square of Fourier coefficients of $x(t)$. Max Born while formulating quantum scattering, arrived at the probabilistic interpretation of the wave function.

15. **Mathematical foundations (1927)** The works of Dirac on classical correspondence, transformation theory, of Hilbert and of von Neumann brought in the Hilbert spaces into quantum mechanics as its mathematical foundation.

16. **Uncertainty principle (1927)** The fact that one could not assign precise values to canonical conjugate pair of variables is implicitly there in Dirac Jordan transformation theory and Dirac and Jordan were aware of this fact. Heisenberg proceeded to formulate this mathematically and arrived at his famous uncertainty principle. Several issues became clear through works of Rurak, Kennard, Condon, Robertson and others before it was established that the uncertainty in the form we understand today.

17. **Complementarity Principle (1928)** Soon after quantum mechanics was fully developed and equivalence of matrix mechanics and wave mechanics was established, questions of interpretation of quantum mechanics were hotly debated. The complementarity principle played an important role in clarifying issues related to the interpretation of quantum mechanics.

Notes and References

[1] For a student of quantum mechanics a strongly recommended book for details of historical account is :
Max Jammer, *The Conceptual Development of Quantum Mechanics*, McGraw-Hill Book Company New York (1966).

[2] The write up on matrix mechanics is based on J. Mehra's account in his Heisenberg memorial lecture at CERN in 1976. This lecture contains details of Heisenberg's contribution and sequence of events in those fateful years. It gives a fascinating accounts of how Heisenberg, and also Born spent sleepless night, before seeing the light in the morning.

Jagdish Mehra, *The Birth of Quantum Mechanics*, Werner Heisenberg Memorial Lecture delivered at the CERN Colloquium on 30 March 1976, CERN Report 76-10.

[3] A brief account of historical development of mathematical foundations of quantum theory can be found in
Arno Bohm, Haydar Uncu and S. Komy, *A Brief Survey of the Mathematics of Quantum Physics*, Reports on Mathematical Physics **64** (2009) 5-32.

Lecture 3

Consequences of wave particle duality

The year 1926 saw quantum mechanics getting established with formalism and rules for computation firmly in place. However, the issues related to the interpretation were unclear and were being hotly debated. The thought experiments played an important role in the debates involving Bohr, Schrodinger, Heisenberg and Einstein and others.

In the next two sections we will briefly discuss a few of these thought experiments which are crucial for understanding the nature of conceptual changes brought in by quantum mechanics. In these discussions the wave particle duality plays an important role in clarifying conceptual issues related to the *uncertainty principle* and *superposition principle* in quantum mechanics.

The wave particle duality has far reaching consequences. Feynman analyses thought experiments on electron beam incident on single and double slit. He also discusses the situation when the intensity of electron beam is reduced so that only one electron is incident at a time.

Dirac, in his classic book presents, a discussion of photon polarization experiment and what happens when one photon is incident at time. He shows that it leads to the principle of superposition of states for photon. Similar conclusions are reached as a result of an analysis of double slit interference of photons.

The inability to consistently describe the outcomes of these experiments in terms of deterministic behaviour of a single particle thus leads to indeterminacy and introduction of probability in quantum theory. The nature and reasons for appearance probabilities in classical and in quantum theory are brilliantly discussed by Feynman and by Dirac.

Dirac also emphasizes how superposition principle for quantum states is different from that for appearing for waves in classical physics.[1]

It is suggested that the reader should go through the original discussions by Dirac [**?**]

[1] Flagged for Adding Excerpts

and Feynman [?] on the thought experiments.

§1 Measurement of position

Measurement using a single slit

Let us consider a beam of electrons incident on a thin slit as shown in the 1. The slit allows only a small width of the beam along the z- axis to pass through, the rest of the beam is blocked. This could be regarded as an arrangement for measurement of the z-component of the position of an electron in the beam. For an electron passing through the slit, the z- component of the position is known upto an accuracy equal to the width of the slit d. Let p be the momentum of the electrons in the beam. Then the wave length associated with the electrons is $\lambda = h/p$. Due to diffraction of the electron waves the electrons, after passing through the slit, will come out diverging at an angle α and z-component of momentum will be uncertain by an amount

$$\Delta p_z \approx p \sin\alpha \tag{3.1}$$

where $\sin\alpha \approx \lambda/d$. Thus

$$\Delta z \Delta p_z \approx d \times (p\sin\alpha) = (p\sin\alpha)\Big(\frac{\lambda}{\sin\alpha}\Big) \tag{3.2}$$

$$\therefore \Delta z \Delta p_z \approx \hbar. \tag{3.3}$$

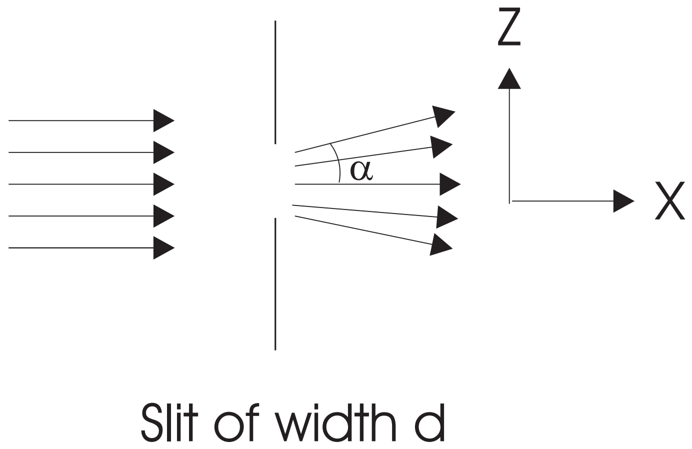

Fig. **1** Measurement of position using single slit

Heisenberg Microscope

Let us consider measurement of position of a point particle by means of a microscope. Let the particle be at a point P and its position be measured by allowing light to fall on the particle and collecting the light scattered from the particle, see 2. The resolving power of the lens, $\lambda/\sin\alpha$, sets the limit on the accuracy upto which the x- component of position, (see Fig.2.2) can be measured. In the process of measurement the photon gets scattered from the particle and, after the scattering, the photon will enter the microscope if it is travelling in a cone of angle α. Thus the x- component of the photon momentum will be uncertain by an amount $p\sin\alpha$, where p is the initial momentum of the photon. This introduces an uncertainty

$$\Delta p_x \approx p\sin\alpha = \frac{h}{\lambda}\sin\alpha \tag{3.4}$$

in the momentum of the particle after the measurement has been made. Thus, we have

$$\Delta x \approx \frac{\lambda}{\sin\alpha}, \qquad \Delta p_x \approx \frac{h}{\lambda}\sin\alpha, \tag{3.5}$$

$$\Delta x \Delta p_x \approx h \tag{3.6}$$

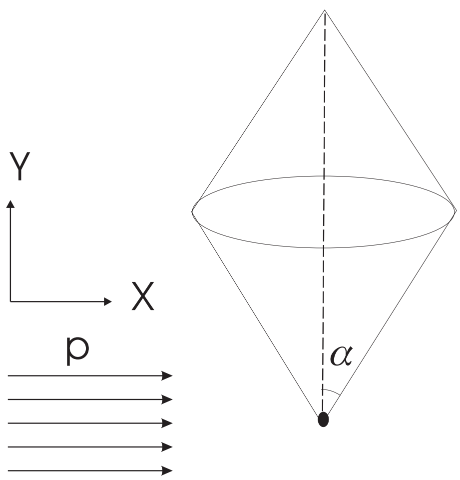

Fig. **2** Heisenberg Microscope

§2 Measurement of momentum

Measurement using Doppler shift

Let us consider an experiment involving measurement of momentum of an atom by measuring the Doppler shift of the radiation emitted by the atom[**?**]. Let ν be the frequency of the radiation emitted by the atom at rest and ν' be the frequency when it is moving with velocity v. Then the nonrelativistic formula for the Doppler shift gives

$$\frac{v}{c} \approx \frac{\nu - \nu'}{\nu} \tag{3.7}$$

The uncertainty in measurement of velocity depends on the accuracy of measurement of ν, which in turn depends on the time τ which is the duration of measurement of the frequency. The error in the frequency measurement is given by $\Delta\nu = 1/\tau$. The time T , when the photon is emitted, can have any value between 0 and τ . When the photon is emitted, the momentum changes abruptly by an amount $\delta p = h\nu'/c$ and the change in velocity is given by $\delta v = \delta p/m = (h\nu')(mc)$. The position becomes uncertain by an amount δvT . Since this time T can have any value between 0 and τ and it cannot be determined, the uncertainty in position will be

$$\Delta x \approx \delta vT \frac{h\nu'\tau}{mc} \tag{3.8}$$

The error in measurement of the momentum, using Eq.(3.7), is given by

$$\Delta p = m\Delta v = \frac{m\Delta\nu'}{c\nu} = \frac{mc}{\tau\nu}. \tag{3.9}$$

Hence, taking $\nu = \nu'$, we get

$$\Delta x\Delta p \approx h. \tag{3.10}$$

Some other thought experiments, that can be analysed for momentum measurement of a charged particle, consist in using of motion in a magnetic field, and measuring the change in wavelength in scattering of photon, Compton effect. In all such experiments one is led to the Heisenberg uncertainty relation as a consequence of wave particle duality. It must be noted that a measurement of position (momentum) gives disturbs momentum (position) of the particle by an amount that is uncontrollable fashion and can not be measured and thereby leading to the uncertainty relation.

Lecture 4

New Concepts Brought in by Quantum Theory A summary

We summarize some important classical concepts which underwent a complete revision after the quantum revolution. We relate these changes to the developments that took place before quantum mechanics was established (1900-1924).This list is aimed to provide a motivation for the postulates of quantum mechanics.

- **Discontinuous nature of physical processes**
  The classical physical processes are perceived as happening continuously. In contrast to the prevailing models, Planck's explanation of black body radiation, Einstein's explanation of photoelectric effect and Bohr model, all assumed that the the process of emission of radiation is discontinuous. Niels Bohr brought in quantum jumps to explain hydrogen atom spectrum.

- **Quantization of dynamical variables**
  In classical theories dynamical variables associated with waves and particles can take continuous values.

  In quantum description, the dynamical variables are quantized, in general, they can take only some discrete values. This was needed for many successful explanations of physical phenomena in days of old quantum theory, Bohr's model being one such example. That all values are not allowed for z- component of angular momentum, was postulated in order to explain Zeeman effect. The Stern Gerlach experiment demonstrated quantization of intrinsic magnetic moment and of spin.

- **Simultaneous measurement**
  Unlike classical theories, in general two arbitrary dynamical variables cannot be measured simultaneously. It has roots in Heisenberg's work that the position and canonical conjugate momentum cannot be measured to arbitrary accuracy simultaneously. Limitations on simultaneous measurement of position and momentum can

be traced back to wave particle duality.

- **Wave particle duality** In classical theory we associate a well defined trajectory with motion of particles. Waves are not localized and one cannot associate definite trajectories with waves. Properties of particles and waves are incompatible properties.

- **Complementarity principle**

  In general, electrons, protons etc. are described by wave packets and have position and momentum defined subject to restrictions imposed by the uncertainty principle.

  A particle description becomes a good approximation in certain regimes such as small wavelength. The wave nature takes over for large wavelengths.

  The two natures are complementary. They are both needed to have a complete understanding of physical systems. The two aspects do not manifest themselves in any single experiment. (Bohr complementarity principle)

- **Quantum tunnelling**
  The classical motion of particle is confined to regions where the total energy is greater than the potential energy. A classical particle cannot cross a region where the potential energy is higher than the kinetic energy. (Barrier tunnelling as in alpha decay.)

  This does not surprise us if we look at the wave picture. The tunnelling through a barrier can be understood in terms of evanescent waves in a medium where the waves can not propagate.

- **Superposition principle**
  Within the classical framework an understanding of the wave phenomena such as interference, diffraction and polarisation require superposition of waves.

  In quantum theory, the wave particle duality also requires a superposition principle. This is *"superposition of states"* as against superposition of wave amplitudes in classical physics. Read more about it from [**?**].

- **States of physical system**
  The states of a quantum system are no longer specified by the generalised coordinates and momenta.

- **Dynamical variables as operators**
  The dynamical variables are no longer ordinary functions of canonical variables.

- **Quantisation as an eigenvalue problem**
  A measurement of a dynamical variable does not give all possible (classically al-

lowed) values. That allowed values are to be computed by solving eigenvalue problem was brought in by works of Schrödinger.

- **Indeterminacy and probability**

  The classical theories are deterministic, where as the quantum theory is probabilistic, again as a consequence of wave particle duality.

  An analysis of thought experiments reveals the indeterministic nature of quantum theory.

  The quantum theory predicts only probabilities of possible outcomes of experiments of measurements.

  Thus a measurement of a dynamical variable yields only probabilities for different possible outcomes of permissible values.

Not only our understanding of classical concepts require a major shift or a complete change and many new concepts are brought in by the quantum theory. In addition entire mathematical framework needed for description of quantum phenomena changes. While the mathematics prerequisite for classical mechanics for solution of problems is differential equations and partial differential equations, quantum mechanics brought in new mathematics. Several possible approaches with variety of starting points are available, the most commonly used one makes use of Hilbert spaces and probability theory in an essential way.

The above description of changes brought by quantum theory is meant to serve as a warning to young readers that a continued attempt to use classical concepts, without care, will result in loss of understanding and seemingly paradoxical situations. It must be remembered that classical mechanics does not become fully obsolete, and that care is required in using classical picture for a given system. In fact correspondence with classical mechanics is capable of providing useful insights and continues to be an active and fertile research area. We end this section with a quote from Landau and Lifshitz [**?**]

> Thus quantum mechanics occupies a very unusual place among physical theories: it contains classical mechanics as a limiting case, yet at the same time it requires this limiting case for its own formulation.

Lecture 5

Schrodinger wave equation

Point Particle	**Waves**
Mass Point	Wave packet
Trajectory	Ray
Velocity,ϑ	Group Velocity,$\tilde{\vartheta}$
	Phase Velocity, (v)
Potential Energy $\vartheta(x)$	Refractive Index,
	Function of position $n(x)$
Energy E	Frequency ν
	Dispersive medium, $n(,\nu,x), v(\nu,x)$
Manupertuis Principle:	Fermat Priniciple:

$$\int \sqrt{E-\vartheta(x)}dx = \min \qquad \int \frac{ds}{v(\nu,x)} = \min$$

Remark Note that,for a particle,$\int \sqrt{E-V(x)dr}$ =min,means $\int pdx = \min$ which, for $E = \text{const}$, implies $\int(pdx - Hdt) = \min$.
Particles have dual nature, therefore consistency requires that both Maupertuis and Fermat principles should give the same answer. Therefore, we must have

$$\frac{1}{v(\nu,x)} = f(\nu)\sqrt{E-V(x)} \tag{5.1}$$

Velocity of a point mass is

$$\nu = \frac{p}{m} = \sqrt{2(E-V(x))/m.} \tag{5.2}$$

and group velocity, for waves, is given by

$$v_g = \frac{d\omega}{dk} = 1/(\frac{dk}{d\omega}) \tag{5.3}$$

Note that $v - \nu\lambda, \omega = 2\pi\nu$ and $k = 2\pi/\lambda$,

$$v_g = 1/\frac{d}{d\nu}(1/\lambda) = 1/\frac{d}{d\nu}(\frac{\nu}{v(\nu)}) \tag{5.4}$$

Thus, for velocity of a mass point, we get

$$\frac{1}{\vartheta} = \frac{d}{d\nu}(\frac{v}{v(v,x)}) \tag{5.5}$$

Velocity of a mass point ϑ corresponds to the group velocity v_g of wave packet $=\tilde{\vartheta}$. Hence

$$\sqrt{\frac{m}{2}}\frac{1}{\sqrt{E - V(x)}} = \frac{d}{d\nu}(\nu f(\nu)\sqrt{E(\nu) - V(x)}) \tag{5.6}$$

$$= \frac{d}{d\nu}(\nu f(\nu))\sqrt{E(\nu) - V(x)} + \frac{\nu f(\nu)}{2}\frac{dE(\nu)}{d\nu}\frac{1}{E(\nu) - V(x)} \tag{5.7}$$

This equation will be correct for all x and all $\vartheta(x)$ if

$$\frac{d}{d\nu}(\nu f(\nu)) = 0 \text{ or } \nu f(\nu) = \text{const,K}. \tag{5.8}$$

and the coefficient of $\frac{1}{\sqrt{E-V(x)}}$ on both sides are equal:

$$\sqrt{\frac{m}{2}} = \frac{\nu f(\nu)}{2}\frac{dE(\nu)}{d\nu} = \frac{K}{2}\frac{dE(\nu)}{d\nu} \tag{5.9}$$

$$\Rightarrow \frac{dE(\nu)}{d\nu} = \text{const}, h \Rightarrow E = h\nu + \text{const.}, \tag{5.10}$$

Setting this last constant to zero gives

$$\boxed{E = h\nu} \tag{5.11}$$

and Eq.(10) determines the constant $K = \frac{\sqrt{(2m)}}{h}$. Also $\nu f(\nu) = K$ along with Eq.(1)implies

$$\frac{1}{v(\nu,x)} = \frac{K}{\nu}\sqrt{E(\nu) - V(x)} = \frac{\sqrt{2m}}{h\nu}\sqrt{E(\nu) - V(x)} \tag{5.12}$$

or

$$\frac{h}{\sqrt{2m(E(\nu) - V(x))}} = \frac{v}{\nu} = \lambda \tag{5.13}$$

This gives

$$\boxed{\lambda = \frac{h}{p}} \tag{5.14}$$

Derivation of Schrdinger Equation For monochromatic waves

$$\nabla^2\psi - \frac{1}{v^2}\frac{d^2\psi}{dt^2} = 0 \tag{5.15}$$

We set $\psi(x,t) = u(x)e^{-i\omega t}$, assuming ω to be fixed, using Eq. (13) we get

$$\nabla^2 u + \frac{\omega^2}{v^2} u = 0 \tag{5.16}$$

$$\Rightarrow \nabla^2 u + \frac{4\pi\nu^2}{h^2\nu^2}(2m(E(\nu) - V(x))u = 0 \tag{5.17}$$

$$\Rightarrow \nabla^2 u + \frac{2m}{h^2}(E(\nu) - V(x))u = 0 \tag{5.18}$$

For states with fixed energy, we have

$$E\psi = h\omega\psi \sim ih\frac{\partial\psi}{\partial t}, \tag{5.19}$$

giving the time dependent Schrdinger equation

$$ih\frac{\partial\psi}{\partial t} = -\frac{h^2}{2m}\nabla^2\psi + V(x)\psi \tag{5.20}$$

Clap!Clap!

Remarks:

The highlight of this route is the derivation of de Broglie relation $\lambda = h/p$ and the Einstein relation $E = h\nu$ for point particles by demanding the action principles for matter and waves give the same result.

I thank Bindu Bambah for providing Fermi's Chicago University lecture notes to me. I wish Fermi's Lecture Notes were available to the present generation of students.