Introduction to Spectral Theory of Linear Operators

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Subsection 1

States, Observables, Position Operator

Classical versus Quantum Mechanics

- Consider a single particle, constrained to one dimension (i.e., $\mathbb{R}$).
- The system is fixed at an arbitrary instant, i.e., time is a parameter which we keep fixed.
  - In classical mechanics, the state of the system at some instant is described by specifying the position and velocity of the particle. Hence, classically, the instantaneous state of the system is described by a pair of numbers.
  - In quantum mechanics, the state of the system is described by a function ψ.
    ψ is complex-valued and is defined on $\mathbb{R}$, i.e., it is a complex function of a single real variable q.
    We assume that ψ is an element of the Hilbert space $L^2(-\infty, +\infty)$.

The Physical Interpretation of ψ

- ψ is related to the probability that the particle will be found in a given subset $J \subseteq \mathbb{R}$,
$$\int_J |\psi(q)|^2 dq.$$
- To the whole one-dimensional space $\mathbb{R}$, there should correspond the probability 1, i.e., we want the particle to be somewhere on the real line
$$\|\psi\|^2 = \int_{-\infty}^{+\infty} |\psi(q)|^2 dq = 1.$$
- The integral $\int_J |\psi(q)|^2 dq$ remains unchanged if we multiply ψ by a complex factor of absolute value 1.

States of the System

- The deterministic description of a state in classical mechanics is replaced by a probabilistic description of a state in quantum mechanics.
- Define a **state** (of our physical system at some instant) to be an element $\psi \in L^2(-\infty, +\infty)$, with $\|\psi\| = 1$.
- More precisely, it is an equivalence class of such elements, where

$$\psi_1 \sim \psi_2 \;\Leftrightarrow\; \psi_1 = \alpha\psi_2,\; |\alpha| = 1.$$

- For the sake of simplicity, we denote these equivalence classes again by letters such as ψ, φ, etc.
- ψ generates a one-dimensional subspace of $L^2(-\infty, +\infty)$,

$$Y = \{\varphi : \varphi = \beta\psi, \beta \in \mathbb{C}\}.$$

  - A **state** of the system is a one-dimensional subspace $Y \subseteq L^2(-\infty, +\infty)$;
  - A probability is computed using a $\varphi \in Y$ of norm 1.

Mean and Expected Value

- $|\psi(q)|^2$ plays the role of the density of a probability distribution on $\mathbb{R}$.
- By definition, the corresponding **mean value** or **expected value** is

$$\mu_\psi = \int_{-\infty}^{+\infty} q|\psi(q)|^2 dq.$$

- The **variance** of the distribution is

$$\text{var}_\psi = \int_{-\infty}^{+\infty} (q-\mu_\psi)^2 |\psi(q)|^2 dq.$$

- The **standard deviation** is

$$\text{sd}_\psi = \sqrt{\text{var}_\psi} \geq 0.$$

The Position Operator

- We can write the mean in the form

$$\mu_\psi(Q) = \langle Q\psi, \psi \rangle = \int_{-\infty}^{+\infty} Q\psi(q)\overline{\psi(q)}dq,$$

  where the operator $Q : \mathscr{D}(Q) \to L^2(-\infty, +\infty)$ is the **multiplication by the independent variable** q, defined by

$$Q\psi(q) = q\psi(q).$$

- Since $\mu_\psi(Q)$ characterizes the average position of the particle, Q is called the **position operator**.
- By definition, $\mathscr{D}(Q)$ consists of all $\psi \in L^2(-\infty, +\infty)$, such that $Q\psi \in L^2(-\infty, +\infty)$.

Position Operator and Variance

- By preceding work, Q is an unbounded self-adjoint linear operator whose domain is dense in $L^2(-\infty,+\infty)$.
- The variance can be written

$$\begin{aligned} \text{var}_\psi(Q) &= \langle (Q-\mu I)^2\psi,\psi\rangle \qquad (\mu=\mu_\psi(Q)) \\ &= \int_{-\infty}^{+\infty}(Q-\mu I)^2\psi(q)\overline{\psi(q)}dq. \end{aligned}$$

Need for Observables

- A state ψ of a physical system contains our entire theoretical knowledge about the system, but only implicitly.
- The problem is how to obtain from a ψ some information about quantities that express properties of the system which we can observe experimentally, called observables.
- Examples of observables are position, momentum and energy.
- In the case of position, we have the self-adjoint linear operator Q.
- This suggests that in the case of other observables, we proceed in a similar fashion, that is, introduce suitable self-adjoint linear operators.

Observables

- Define an **observable** (of our physical system at some instant) to be a self-adjoint linear operator $T:\mathscr{D}(T)\to L^2(-\infty,+\infty)$, where $\mathscr{D}(T)$ is dense in the space $L^2(-\infty,+\infty)$.
- Define the **mean value** $\mu_\psi(T)$ by

$$\mu_\psi(T)=\langle T\psi,\psi\rangle=\int_{-\infty}^{+\infty}T\psi(q)\overline{\psi(q)}dq.$$

- Define the **variance** $\mathrm{var}_\psi(T)$ by

$$\begin{aligned}\mathrm{var}_\psi(T) &= \langle (T-\mu I)^2\psi,\psi\rangle \qquad (\mu=\mu_\psi(T))\\ &= \int_{-\infty}^{+\infty}(T-\mu I)^2\psi(q)\overline{\psi(q)}dq.\end{aligned}$$

Observables (Cont'd)

- Define the **standard deviation** by

$$\mathrm{sd}_\psi(T) = \sqrt{\mathrm{var}_\psi(T)}.$$

- In an experiment, if the system is in state ψ:
  - $\mu_\psi(T)$ characterizes the average value of the observable T;
  - The variance $\mathrm{var}_\psi(T)$ characterizes the variability about the mean.

Subsection 2

Momentum Operator. Heisenberg Uncertainty Principle

The Position and the Momentum Operators

- Consider the same physical system with the position operator

$$\begin{array}{rcl} Q: \ \mathscr{D}(Q) & \to & L^2(-\infty,+\infty); \\ \psi & \mapsto & q\psi. \end{array}$$

- Another very important observable is the momentum p, given by the **momentum operator**:

$$\begin{array}{rcl} D: \ \mathscr{D}(D) & \to & L^2(-\infty,+\infty); \\ \psi & \mapsto & \frac{h}{2\pi i}\frac{d\psi}{dq}, \end{array}$$

  where h is Planck's constant.
- The domain $\mathscr{D}(D) \subseteq L^2(-\infty,+\infty)$ consists of all functions $\psi \in L^2(-\infty,+\infty)$, such that:
  - ψ is absolutely continuous on every compact interval on $\mathbb{R}$;
  - $D\psi \in L^2(-\infty,+\infty)$.

Motivation for the Momentum Operator

- By Einstein's mass-energy relationship $E = mc^2$ (c the speed of light), an energy E has mass $m = \frac{E}{c^2}$.
- Since a photon has speed c and energy $E = h\nu$ (ν the frequency), it has momentum

$$\begin{aligned} p &= mc \quad (\text{mass} \times \text{speed}) \\ &= \frac{h\nu}{c} \\ &= \frac{h}{\Lambda} \quad (\Lambda \text{ the wavelength}) \\ &= \frac{h}{2\pi} k. \quad \left(k = \frac{2\pi}{\Lambda}\right) \end{aligned}$$

- Adopting de Broglie's concept of **matter waves**, satisfying relationships that hold for light waves, we may use the displayed equation also in connection with particles.

State and Fourier Transform

- Assuming the state ψ of our physical system to be such that we can apply the classical Fourier integral theorem, we have

$$\psi(q) = \frac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} \varphi(p) e^{(2\pi i/h)pq} dp.$$

- Here,

$$\varphi(p) = \frac{1}{\sqrt{h}} \int_{-\infty}^{+\infty} \psi(q) e^{-(2\pi i/h)pq} dq.$$

- Physically this can be interpreted as a representation of ψ in terms of functions of constant momentum p given by

$$\psi_p(q) = \varphi(p) e^{(2\pi i/h)pq} = \varphi(p) e^{ikq},$$

where $k = \frac{2\pi p}{h}$ and $\varphi(p)$ is the amplitude.

Fourier Transform and Momentum

- The complex conjugate $\overline{\psi_p}$ has a minus sign in the exponent.
- So, we have

$$|\psi_p(q)|^2 = \psi_p(q)\overline{\psi_p(q)} = \varphi(p)\overline{\varphi(p)} = |\varphi(p)|^2.$$

- Thus, $|\varphi(p)|^2$ must be proportional to the density of the momentum.
- The constant of proportionality is 1, since we have defined $\varphi(p)$ so that the same constant $\frac{1}{\sqrt{h}}$ is involved.

Mean Value of the Momentum

- The mean value of the momentum, call it $\widetilde{\mu}_\psi$, is

$$\begin{aligned}\widetilde{\mu}_\psi &= \int_{-\infty}^{+\infty} p|\varphi(p)|^2 dp \\ &= \int_{-\infty}^{+\infty} p\varphi(p)\overline{\varphi(p)}dp \\ &= \int_{-\infty}^{+\infty} p\varphi(p)\frac{1}{\sqrt{h}}\int_{-\infty}^{+\infty}\overline{\psi(q)}e^{(2\pi i/h)pq}dqdp.\end{aligned}$$

- Suppose that:
  - We may interchange the order of integration;
  - In the Fourier transform we may differentiate under the integral sign.
- Then, we obtain

$$\begin{aligned}\widetilde{\mu}_\psi &= \int_{-\infty}^{+\infty}\overline{\psi(q)}\int_{-\infty}^{+\infty}\varphi(p)\frac{1}{\sqrt{h}}pe^{(2\pi i/h)pq}dpdq \\ &= \int_{-\infty}^{+\infty}\overline{\psi(q)}\frac{h}{2\pi i}\frac{d\psi(q)}{dq}dq.\end{aligned}$$

Mean Value of the Momentum and the Momentum Operator

- We obtained
$$\widetilde{\mu}_\psi = \int_{-\infty}^{+\infty} \overline{\psi(q)} \frac{h}{2\pi i} \frac{d\psi(q)}{dq} dq.$$
- Denoting $\widetilde{\mu}_\psi$ by $\mu_\psi(D)$, we can write this in the form
$$\mu_\psi(D) = \langle D\psi, \psi\rangle = \int_{-\infty}^{+\infty} D\psi(q)\overline{\psi(q)} dq.$$
- This motivates the definition of the momentum operator
$$\begin{array}{rccl} D: & \mathscr{D}(D) & \to & L^2(-\infty, +\infty); \\ & \psi & \mapsto & \frac{h}{2\pi i}\frac{d\psi}{dq}. \end{array}$$

The Commutator of Self-Adjoint Operators

- Let S and T be any self-adjoint linear operators with domains in the same complex Hilbert space.
- Then the operator
$$C = ST - TS$$
is called the **commutator** of S and T.
- The commutator C of S and T is defined on
$$\mathscr{D}(C) = \mathscr{D}(ST) \cap \mathscr{D}(TS).$$

The Commutator of the Position and the Momentum

- By straightforward differentiation we have

$$DQ\psi(q) = D(q\psi(q)) = \frac{h}{2\pi i}[\psi(q) + q\psi'(q)] = \frac{h}{2\pi i}\psi(q) + QD\psi(q).$$

- This gives the **Heisenberg commutation relation**

$$DQ - QD = \frac{h}{2\pi i}\widetilde{I},$$

where $\widetilde{I}$ is the identity operator on the domain

$$\mathscr{D}(DQ - QD) = \mathscr{D}(DQ) \cap \mathscr{D}(QD).$$

- The domain $\mathscr{D}(DQ - QD)$ is dense in the space $L^2(-\infty, +\infty)$.

  It contains the sequence (e_n) of the Hermite polynomials, which is total in $L^2(-\infty, +\infty)$.

The Commutator Theorem

Theorem (Commutator)

Let S and T be self-adjoint linear operators with domain and range in $L^2(-\infty,+\infty)$. Then $C = ST - TS$ satisfies

$$|\mu_\psi(C)| \le 2\mathrm{sd}_\psi(S)\mathrm{sd}_\psi(T),$$

for every ψ in the domain of C.

- Write $\mu_1 = \mu_\psi(S)$, $\mu_2 = \mu_\psi(T)$, $A = S - \mu_1 I$ and $B = T - \mu_2 I$. We have

$$\begin{aligned} C = ST - TS &= (A+\mu_1 I)(B+\mu_2 I) - (B+\mu_2 I)(A+\mu_1 I) \\ &= AB + \mu_1 B + \mu_2 A + \mu_1\mu_2 I - BA - \mu_1 B - \mu_2 A - \mu_1\mu_2 I \\ &= AB - BA. \end{aligned}$$

  By hypothesis, S and T are self-adjoint. Since μ_1 and μ_2 are inner products, they are real. Hence A and B are self-adjoint.

The Commutator Theorem (Cont'd)

- By definition,

$$\begin{array}{rcl}\mu_\psi(C) & = & \langle (AB-BA)\psi,\psi\rangle \\ & = & \langle AB\psi,\psi\rangle - \langle BA\psi,\psi\rangle \\ & = & \langle B\psi, A\psi\rangle - \langle A\psi, B\psi\rangle.\end{array}$$

The last two products are equal in absolute value.

Hence, by the triangle and Schwarz inequalities, we have

$$|\mu_\psi(C)| \le |\langle B\psi, A\psi\rangle| + |\langle A\psi, B\psi\rangle| \le 2\|B\psi\|\|A\psi\|.$$

Since B is self-adjoint,

$$\|B\psi\| = \langle (T-\mu_2 I)^2\psi,\psi\rangle^{1/2} = \sqrt{\mathrm{var}_\psi(T)} = \mathrm{sd}_\psi(T).$$

Similarly for $\|A\psi\|$.

Heisenberg Uncertainty Principle

Theorem (Heisenberg Uncertainty Principle)

For the position operator Q and the momentum operator D,

$$\mathrm{sd}_\psi(D)\mathrm{sd}_\psi(Q) \geq \frac{h}{4\pi}.$$

- By the Heisenberg Commutation Relation, $C := DQ - QD = \frac{h}{2\pi i}\widetilde{I}$.

  Hence,

  $$|\mu_\psi(C)| = |\langle C\psi, \psi\rangle| = \left\langle \frac{h}{2\pi i}\widetilde{I}\psi, \psi \right\rangle = \frac{h}{2\pi}.$$

  By the Commutator Theorem, we get

  $$\frac{h}{4\pi} = \frac{1}{2}|\mu_\psi(C)| \leq \mathrm{sd}_\psi(D)\mathrm{sd}_\psi(Q).$$

Interpretation of the Heisenberg Uncertainty Principle

- The standard deviation $\text{sd}_\psi(D)$ characterizes the precision of the measurement of the momentum.
- The standard deviation $\text{sd}_\psi(Q)$ characterizes the precision of the measurement of the position.
- So the inequality

$$\text{sd}_\psi(D)\text{sd}_\psi(Q) \geq \frac{h}{4\pi}$$

means that we cannot make a simultaneous measurement of position and momentum of a particle with an unlimited accuracy.

Subsection 3

Time-Independent Schrodinger Equation

The Wave Equation

- For investigating refraction, interference and other more subtle optical phenomena one uses the **wave equation**

$$\Psi_{tt} = \gamma^2 \Delta \Psi,$$

  where:
  - $\Psi_{tt} = \frac{\partial^2 \Psi}{\partial t^2}$;
  - The constant γ^2 is positive;
  - $\Delta \Psi$ is the Laplacian of Ψ.
- If q_1, q_2, q_3 are Cartesian coordinates in space, then

$$\Delta \Psi = \frac{\partial^2 \Psi}{\partial q_1^2} + \frac{\partial^2 \Psi}{\partial q_2^2} + \frac{\partial^2 \Psi}{\partial q_3^2}.$$

- In the system considered in the last section we have only one coordinate, q, and $\Delta \Psi = \frac{\partial^2 \Psi}{\partial q^2}$.

The Helmholtz Equation

- Assume a simple and periodic time dependence, say,

$$\Psi(q_1,q_2,q_3,t)=\psi(q_1,q_2,q_3)e^{-i\omega t}.$$

- Substitute into $\Psi_{tt}=\gamma^2\Delta\Psi$,

$$-\psi\omega^2 e^{-i\omega t}=\gamma^2\Delta\psi e^{-i\omega t}.$$

- Drop the exponential factor and rearrange

$$\Delta\psi+\frac{\omega^2}{\gamma^2}\psi=0.$$

This is the **Helmholtz equation** (time-independent wave equation)

$$\Delta\psi+k^2\psi=0,$$

where

$$k=\frac{\omega}{\gamma}=\frac{2\pi\nu}{\gamma}=\frac{2\pi}{\Lambda}.$$

The Time-Independent Schrödinger Equation

- For Λ we choose the de Broglie wave length of matter waves

$$\Lambda = \frac{h}{mv}.$$

- Then we get $k^2 = \frac{4\pi^2 m^2 v^2}{h^2}$ and

$$\Delta\psi + \frac{8\pi^2 m}{h^2} \cdot \frac{mv^2}{2}\psi = 0.$$

- Let $E = \frac{mv^2}{2} + V$ be the sum of the kinetic and the potential energy.
- Then we can write

$$\Delta\psi + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0.$$

- This is the famous **time-independent Schrödinger equation**.

Schrödinger Equation and Bohr's Theory

- Rewrite $\Delta\psi + \frac{8\pi^2 m}{h^2}(E - V)\psi = 0$ in the form
$$\left(-\frac{h^2}{8\pi^2 m}\Delta + V\right)\psi = E\psi.$$
- This form suggests that the possible energy levels of the system will depend on the spectrum of the operator defined by the left-hand side.
- Physically meaningful solutions of a differential equation should remain finite and approach zero at infinity.
- A potential field being given, Schrödinger's equation has such solutions only for certain values of the energy E.
- They are related to Bohr's theory of the atom in one of two ways:
  - They are in agreement with the "permissible" energy levels of Bohr's theory;
  - They disagree, but they are in better agreement with experimental results than values predicted Bohr's theory.
- So Schrödinger's equation both "explains" and improves Bohr's theory.

Subsection 4

Hamilton Operator

Hamilton Function in Classical Mechanics

- In classical mechanics, one can base the investigation of a conservative system of particles on the **Hamilton function** of the system, i.e., the total energy
$$H = E_{\text{kin}} + V$$
(E_{kin} = kinetic energy, V = potential energy) expressed in terms of position coordinates and momentum coordinates.
- Assuming that the system has n degrees of freedom, one has:
  - n position coordinates $q_1, \ldots, q_n$;
  - n momentum coordinates $p_1, \ldots, p_n$.

Adaptation to Quantum Mechanics

- In the quantum mechanical treatment of the system we also determine

$$H(p_1,\ldots,p_n;q_1,\ldots,q_n).$$

- We then replace each p_j by the momentum operator

$$D_j:\mathscr{D}(D_j)\to L^2(\mathbb{R}^n);\quad \psi\mapsto\frac{h}{2\pi i}\frac{\partial\psi}{\partial q_j},\quad \text{where } \mathscr{D}(D_j)\subseteq L^2(\mathbb{R}^n).$$

- Furthermore, we replace each q_j by the position operator

$$Q_j:\mathscr{D}(Q_j)\to L^2(\mathbb{R}^n);\quad \psi\mapsto q_j\psi,\quad \text{where } \mathscr{D}(Q_j)\subseteq L^2(\mathbb{R}^n).$$

Hamilton Operator in Quantum Mechanics

- The **Hamilton operator**, denoted $\mathscr{H}$, becomes

$$\mathscr{H}(D_1,\dots,D_n;Q_1,\dots,Q_n) := H(p_1,\dots,p_n;q_1,\dots,q_n),$$

  with:
  - p_j replaced by D_j;
  - q_j replaced by Q_j.
- By definition, $\mathscr{H}$ is self-adjoint.
- This process of replacement is called the **quantization rule**.
- The process is not unique (multiplication not commutative).

The Schrödinger Equation with the Hamilton Operator

- The kinetic energy of a particle of mass m in space gives

$$\frac{m}{2}|v|^2 = \frac{m}{2}(v_1^2 + v_2^2 + v_3^2) = \frac{1}{2m}(p_1^2 + p_2^2 + p_3^2).$$

- By the quantization rule the expression on the right yields

$$\frac{1}{2m}\sum_{j=1}^{3} D_j^2 = \frac{1}{2m}\left(\frac{h}{2\pi i}\right)^2 \sum_{j=1}^{3} \frac{\partial^2}{\partial q_j^2} = -\frac{h^2}{8\pi^2 m}\Delta.$$

- Now the equation $(-\frac{h^2}{8\pi^2 m}\Delta + V)\psi = E\psi$ can be written

$$\mathscr{H}\psi = \lambda\psi,$$

where $\lambda = E$ is the energy.

Eigenvalues of the Schrödinger Equation

- We wrote $\mathscr{H}\psi = \lambda\psi$, with $\mathscr{H} = -\frac{h^2}{8\pi^2 m}\Delta + V$ and $\lambda = E$.
  - If λ is in the resolvent set of $\mathscr{H}$, then the resolvent of $\mathscr{H}$ exists and the equation has only the trivial solution, considered in $L^2(\mathbb{R}^n)$.
  - If λ is in the point spectrum $\sigma_p(\mathscr{H})$, then the equation has nontrivial solutions $\psi \in L^2(\mathbb{R}^n)$.
  - The residual spectrum $\sigma_r(\mathscr{H})$ is empty since $\mathscr{H}$ is self-adjoint.
  - If $\lambda \in \sigma_c(\mathscr{H})$, the continuous spectrum of $\mathscr{H}$, then the equation has no solution $\psi \in L^2(\mathbb{R}^n)$, where $\psi \neq 0$.
    However, in this case, it may have nonzero solutions which are not in $L^2(\mathbb{R}^n)$ and depend on a parameter with respect to which we can perform integration to obtain a $\psi \in L^2(\mathbb{R}^n)$.
    In physics, we say that in this process of integration we form **wave packets**.

Free Particle of Mass m on $(-\infty, +\infty)$

- We consider a free particle of mass m on $(-\infty, +\infty)$.
- The Hamilton function is $H(p,q) = \frac{1}{2m}p^2$.
- So the Hamilton operator is

$$\mathscr{H}(D,Q) = \frac{1}{2m}D^2 = -\frac{h^2}{8\pi^2 m}\frac{d^2}{dq^2}.$$

- Hence,

$$\mathscr{H}\psi = -\frac{h^2}{8\pi^2 m}\psi'' = \lambda\psi, \quad \lambda = E \text{ is the energy.}$$

- Solutions are given by

$$\eta(q) = e^{-ikq},$$

where the parameter k is related to the energy by $\lambda = E = \frac{h^2 k^2}{8\pi^2 m}$.

The Fourier-Plancherel Theorem

- These functions η can now be used to represent any $\psi \in L^2(-\infty, +\infty)$ as a wave packet in the form

$$\psi(q) = \frac{1}{\sqrt{2\pi}} \lim_{a \to -\infty} \int_{-a}^{a} \varphi(k) e^{-ikq} dk,$$

where

$$\varphi(k) = \frac{1}{\sqrt{2\pi}} \lim_{b \to \infty} \int_{-b}^{b} \psi(q) e^{ikq} dq.$$

- The limits are in the norm of $L^2(-\infty, +\infty)$ (with respect to q and k, respectively).
- Such a limit is also called a **limit in the mean**.
- The formulas together with the underlying assumptions are called the **Fourier-Plancherel Theorem**.

Free Particle of Mass m in Three Dimensions

- We have
$$\mathscr{H}\psi = -\frac{h^2}{8\pi^2 m}\Delta\psi = \lambda\psi, \quad \Delta \text{ the Laplacian.}$$
- Solutions are plane waves
$$\eta(q) = e^{-ik\cdot q},$$
where $q = (q_1, q_2, q_3)$, $k = (k_1, k_2, k_3)$, and
$$k \cdot q = k_1 q_1 + k_2 q_2 + k_3 q_3.$$
- The energy is
$$\lambda = E = \frac{h^2}{8\pi^2 m} k \cdot k.$$

Free Particle of Mass m in Three Dimensions (Cont'd)

- For a $\psi \in L^2(\mathbb{R}^3)$ the Fourier-Plancherel theorem gives

$$\psi(q) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \varphi(k) e^{-ik\cdot q} dk,$$

where

$$\varphi(k) = \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \psi(q) e^{ik\cdot q} dq.$$

- The integrals are again understood as limits in the mean of corresponding integrals over finite regions in 3-space.

Subsection 5

Time-Dependent Schrodinger Equation

Nonstationary States

- A **stationary state** of a physical system is a state which depends on time only by an exponential factor, say, $e^{-i\omega t}$.
- Other states are called **nonstationary states**.
- The differential equation that such a general function φ of the p_j's, q_j's and t should satisfy cannot be of the form $\Psi_{tt} = \gamma^2 \Delta \Psi$.
  - This is due to the requirement that the function φ be determined for all t if it is given at some instant t.
  - The equation $\Psi_{tt} = \gamma^2 \Delta \Psi$ involves the second derivative with respect to t, and so it leaves the first derivative undetermined.

The Time-Dependent Schrödinger Equation

- The **time-dependent Schrödinger equation** is
$$\mathscr{H}\varphi = -\frac{h}{2\pi i}\frac{\partial\varphi}{\partial t}.$$
- Since it involves i, a nonzero solution φ must be complex.
- $|\varphi|^2$ is regarded as a measure of the intensity of the wave.
- A **stationary solution**, whose intensity at a point is independent of t, is obtained by setting
$$\varphi = \psi e^{-i\omega t},$$
where ψ does not depend on t, and $\omega = 2\pi\nu$.
- Substitution gives
$$\mathscr{H}\psi = -\frac{h}{2\pi i}(-2\pi i\nu)\psi = h\nu\psi.$$
- Since $E = h\nu$, $\mathscr{H}\psi = \lambda\psi$, where $\lambda = E$ is the energy of the system.
- This agrees with the preceding case.