(1)

$\underline{X}$ . . . . $(x_1 . x_2 . . . . x_N)$

$x_1(t=0)$
$\dot{x}_2(t=0)$ . . .
⋮

$\ddot{X}_N = \Sigma' f_{ji} / m$

all initial conditions . . . solve 2. order equation
(analytic solutions) . . . not so often

X, $F(x)$; $\ddot{x} = F(x)/m$

$x(t)$ / $\boxed{F(x) = -k.x}$

$x(t) = C.\cos(\sqrt{\frac{k}{m}}.t)$

$\dot{X} = v$ $\quad (\dot{x} = v$

$\dot{v} = F(x)/m$

$$\frac{d}{dt}\begin{pmatrix} X \\ v \end{pmatrix} = M(x,t)\begin{pmatrix} x \\ v \end{pmatrix}$$

$$M(x,t) = \begin{pmatrix} 0 & 1 \\ -k/m & 0 \end{pmatrix} \qquad Y \equiv \begin{pmatrix} x \\ v \end{pmatrix}$$

$$\frac{d}{dt} Y = \begin{pmatrix} 0 & 1 \\ -\frac{k}{m} & 0 \end{pmatrix} Y$$

Euler's (stupid) method

$$\frac{\Delta X}{\Delta t} \propto F(X,t)$$

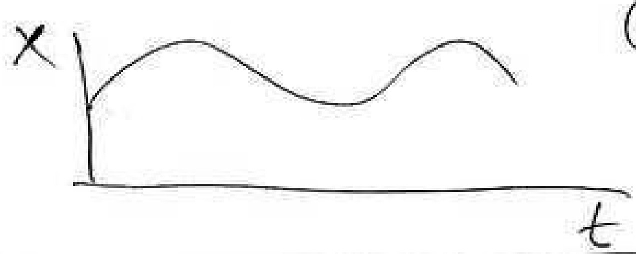
$$\Delta X \simeq F(x,t).\Delta t$$

$X_0(t_0)$; $\Delta X_0 = F(\dots)\Delta t$

$X_1(t_1) = F \dots (t_1 - t_0) + X_0(t_0)$

Runge-Kutta 4-order method (in the computers)

2



trajectory

Schrödinger equation

$\Psi(x,t)$

$\vec{r} = (x,y,z)$

Hamilton

$T + V$

$T = \frac{p^2}{2m}$

Wave mechanics
Matrix mechanics
Dirac notation
Abstract Q. M.
$|\psi\rangle$ bra|ket
$\langle \; | \; \rangle$ Hilbert

δ - function

$\vec{p} = (m\dot{x}, m\dot{y}, m\dot{z})$

$F = -kx \qquad V(x) = \frac{1}{2}kx^2$

$\vec{F} = -\nabla V$

$e^{ikx - i\omega t}$ $\qquad \hbar k = p$

$p_x = -i\hbar \frac{d}{dx}$

$\frac{p_x}{\hbar} \; . \; . \; . \; k \qquad E = \hbar\omega$

$-i\frac{d}{dx}$

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(x)\Psi = i\hbar\frac{\partial}{\partial t}\Psi$$

$i\hbar\frac{\partial}{\partial t}$

$\psi(\vec{x}) \cdot \mathcal{E}(t)$

$i\hbar\frac{\partial}{\partial t}\mathcal{E} = C \cdot \mathcal{E}$ $\qquad \frac{\Psi(x,t)}{\psi(\vec{x})}$

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\psi + V(x)\psi = C\psi}$$

$C = E$ energy

$$L\psi = M\psi$$ (3)

$\psi(x,y)$

if $L(x)$, $M(y)$ (see ... $\frac{\partial}{\partial t}$ ... $M(t)$; ∇ ... $L(x)$)

assume $\psi(x,y) = X(x)\,Y(y)$

$$(LX)Y = (MY)X$$

$$\underbrace{\frac{1}{X} LX}_{\text{no } x} = \underbrace{\frac{1}{Y} MY}_{\text{no } y} = C$$

Exercises

$x, y, z.$ $\quad r = \sqrt{x^2+y^2+z^2}$ $\quad$ $0,0,0$ $\quad r$

$\vartheta \quad (0, \pi)$

$\varphi \quad (0 \dots 2\pi)$

$$\nabla^2 \equiv \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \qquad L^2$$

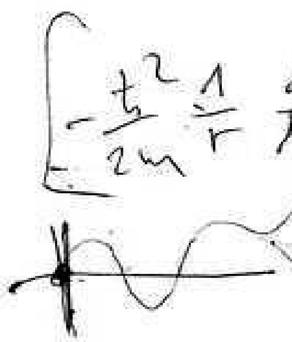
$$\nabla^2 \longrightarrow \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + (\text{horrible } \vartheta, \varphi)$$

$$\psi(r, \vartheta, \varphi) = R(r)\, Y(\vartheta, \varphi)$$

isotropic solution $L^2 Y = 0 \cdot Y$

(in fact not depend on ϑ, φ)

$$\left[-\frac{\hbar^2}{2m} \frac{1}{r} \frac{d}{dr} r \frac{d}{dr} + V(r) \right] R(r) = E\, R(r)$$



$$r\,R(r) = u(r) \qquad -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} u(r) + V(r)\,u = E\,u$$

$\underline{\underline{|\psi(\vec{x})|^2}} = P(x)$ 4 probability density

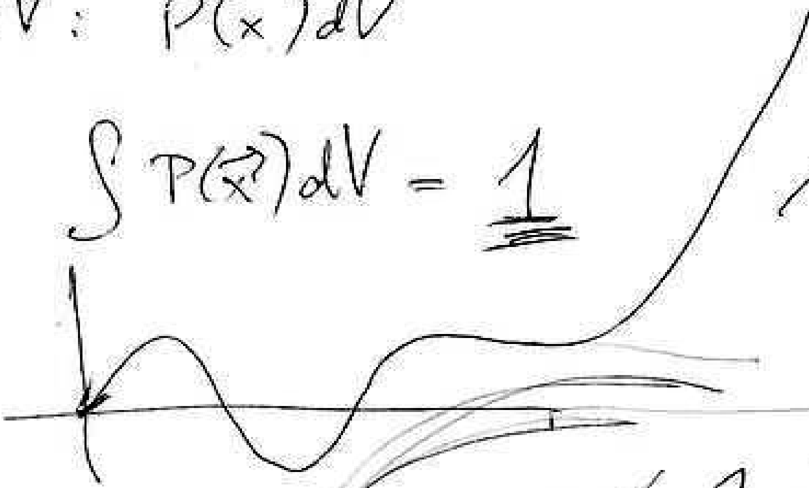
$dV: \quad P(x)\,dV$

dV

$\vec{x} \quad P(\vec{x})$

$dV = d^3\vec{x}$

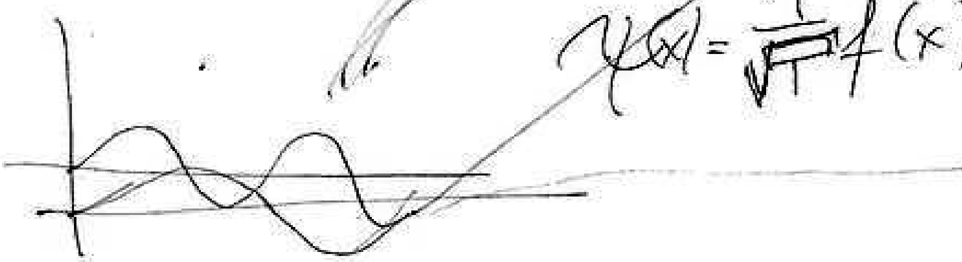
$$\int P(\vec{x})\,dV = \underline{\underline{1}}$$



$$\int |f(x)|^2 dx = I$$

$$\psi(x) = \frac{1}{\sqrt{I}} f(x) \quad \longleftrightarrow \text{normaliz}$$

$$\int |\psi(x)|^2 = 1$$



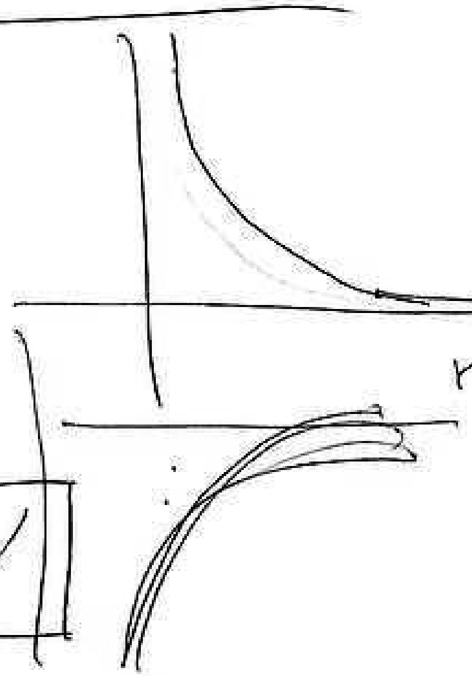
$$a + 7 = 12$$

$-k\cancel{x} \quad \dots \quad \frac{1}{2}kx^2$

$\frac{1}{r^2} \quad \dots \quad +\frac{1}{r}$

$-\frac{1}{r^2} \quad \quad -\frac{1}{r}$

$-\frac{1}{n^2}E_0 \quad \quad \boxed{E_0 = 13.6\,eV}$

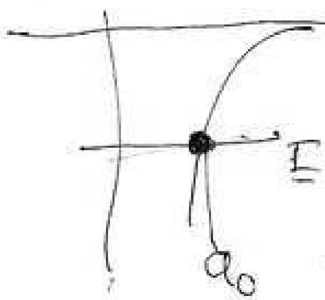


ATOMIC UNITS (5)

$a_0 = 0.529\ \text{Å} = 0.529 \cdot 10^{-10}\ m$

e ... electron charge

$\left(\frac{1}{r} \right.$



$\frac{e^2}{r}$ $\left(\frac{e^2}{4\pi\varepsilon_0 r} \right.$

$\frac{e^2}{a_0}$

Virial theorem

$|\langle T \rangle| = \left(\frac{1}{2}\right) \langle V \rangle$

$T = \frac{1}{2} \frac{\hbar^2 k_0^2}{m}$

$k_0 = \frac{1}{a_0}$

$\langle T \rangle = \frac{1}{2} \frac{\hbar^2}{2 m a_0^2}$

$\frac{1}{2} \langle V \rangle = \frac{1}{2} \frac{e^2}{a_0}$

$\frac{\hbar^2}{m a_0^2} = \frac{e^2}{a_0}$

$+E_0 = \left(\frac{1}{2} \frac{e^2}{a_0} = \frac{me^4}{\hbar^2} \right)$

$\frac{\hbar^2}{m a_0} = e^2$

$E_0 = \left(\frac{1}{2} \frac{e^2}{a_0} \right) = \left(\frac{1}{2} \frac{me^4}{\hbar^2} \right)$

$\boxed{a_0 = \frac{\hbar^2}{me^2}}$

$\underline{\underline{\hbar}}$ $\frac{e^2}{a_0}$

$\underline{(\text{Action}}$ E time

$(10^{-16}$

eVs : $\hbar$ $1 \cdot 10^{-15}$ eVs

$1\,eV \approx 1.6 \cdot 10^{-19}\,J$

$\underline{\underline{eV}}$

$\frac{\hbar}{E_0}$

$t_0 \approx 10^{-16}\,s$