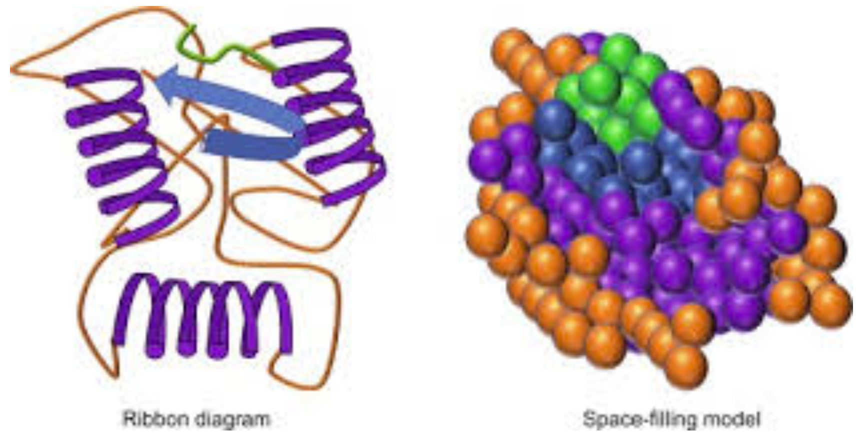
AI and Compex Dynamical Systems

G. P. Tsironis
Department of Physics, University of Crete, Greece

Lecture 1, Friday 18 February 2022

Complex systems

Metals



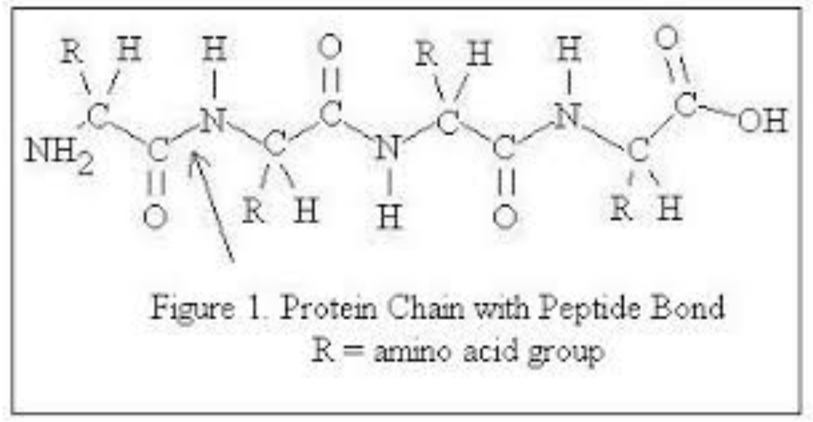


Figure 1. Protein Chain with Peptide Bond
R = amino acid group

Proteins

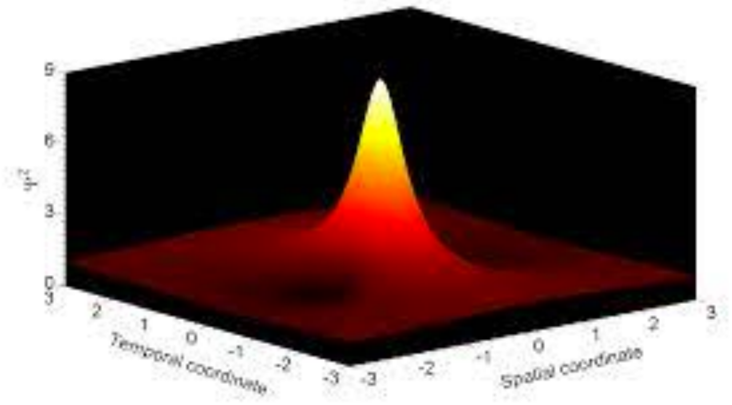
Nonlinear systems

Chaos

Sensitive dependence on initial conditions

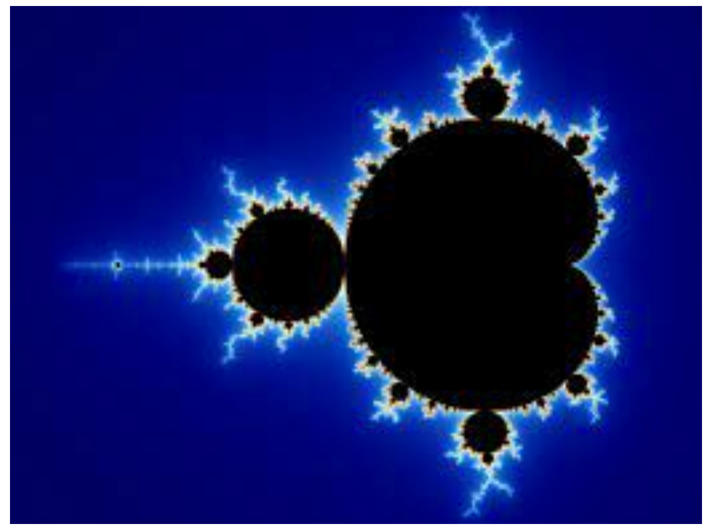
Solitons

Coherent propagation



Fractals

Non-integer dimensional spaces



Chaos

$$\frac{dx}{dt} = \sigma(y - x)$$
$$\frac{dy}{dt} = x(\rho - y) - y$$
$$\frac{dz}{dt} = xy - \beta z$$

4

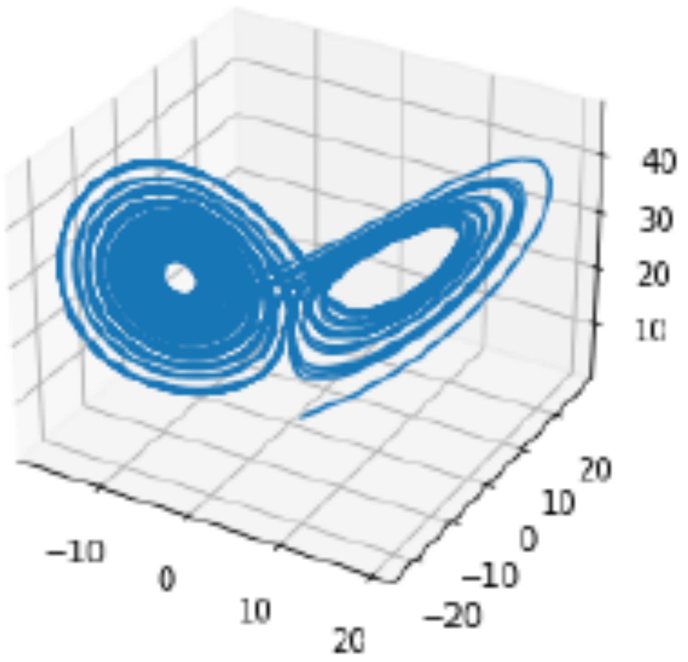
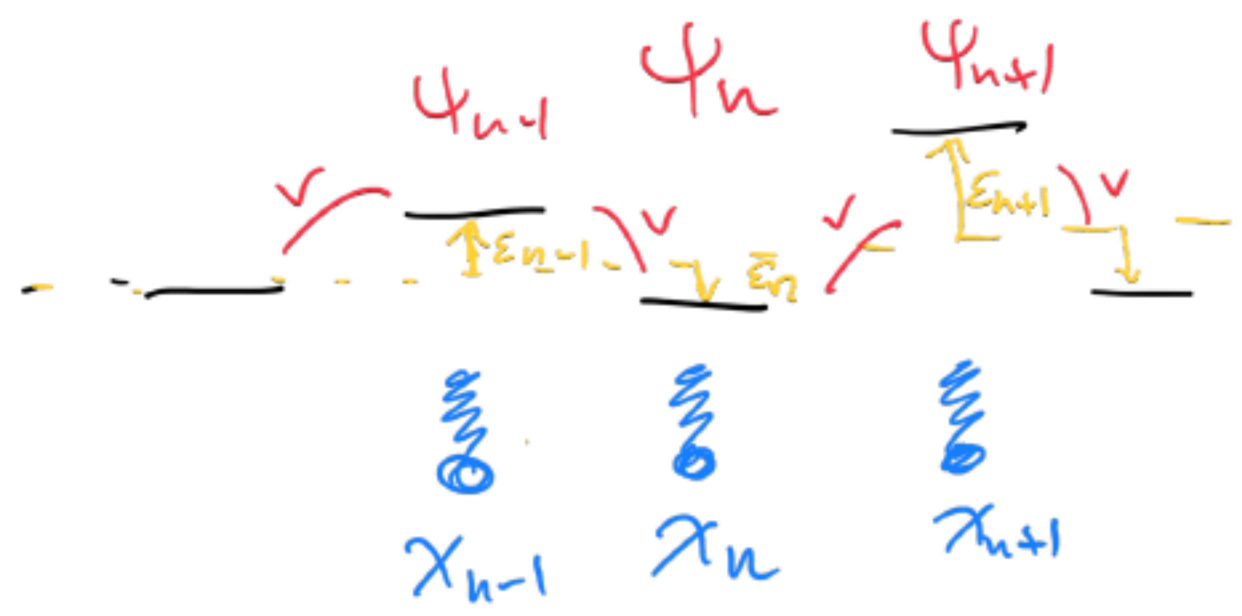


Figure 1: The Lorenz (strange) attractor is a surface with fractal Hausdorff dimension equal to 2.0627160, i.e. it slightly larger than 2. A trajectory that on this attractor moves continuously between the two lobes without a predictable character. In this figure $\rho = 28.0$, $\sigma = 10.0$ and $\beta = 8.0/3.0$

The DNLS equation

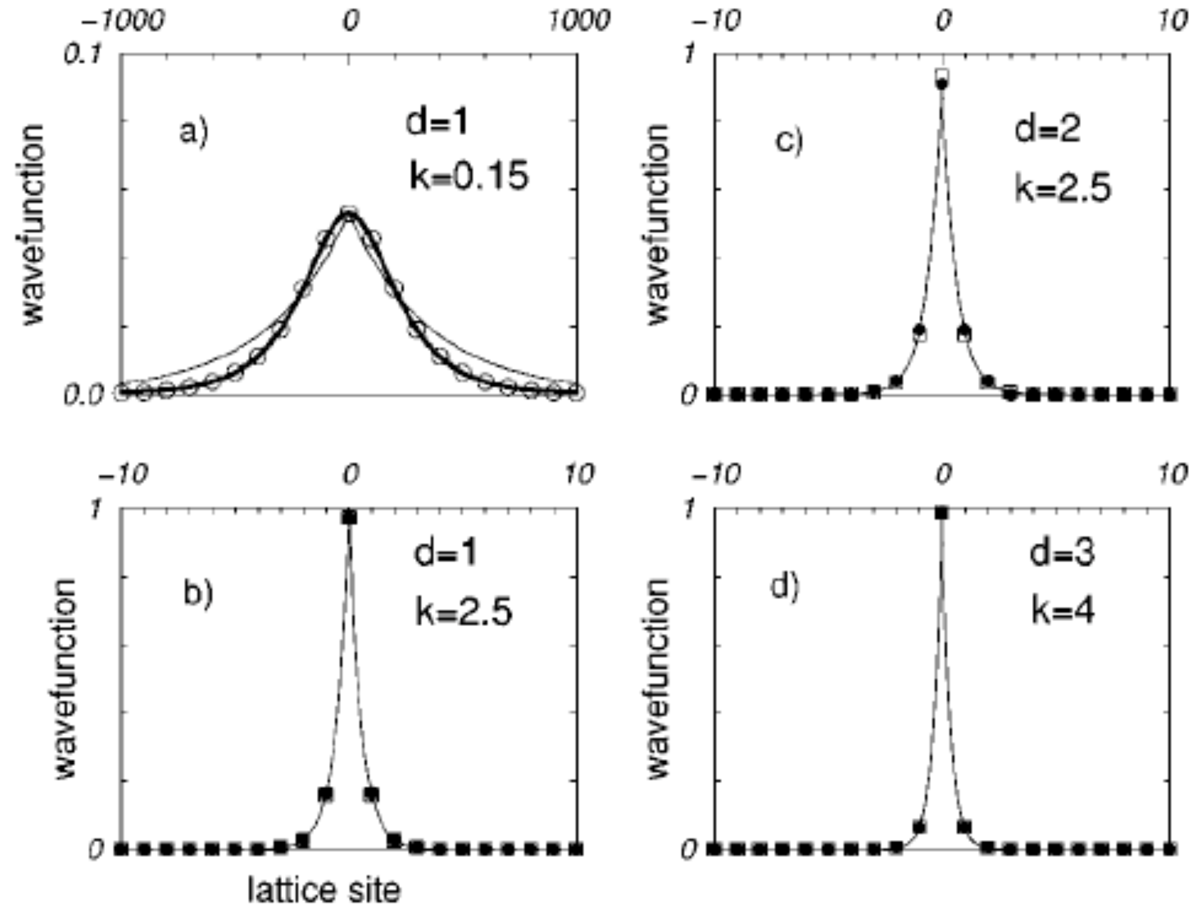
$$i\frac{d\psi_n}{dt} = \epsilon_n \psi_n + V\left(\psi_{n-1} + \psi_{n+1}\right) - \chi_n |\psi_n|^2 \psi_n$$



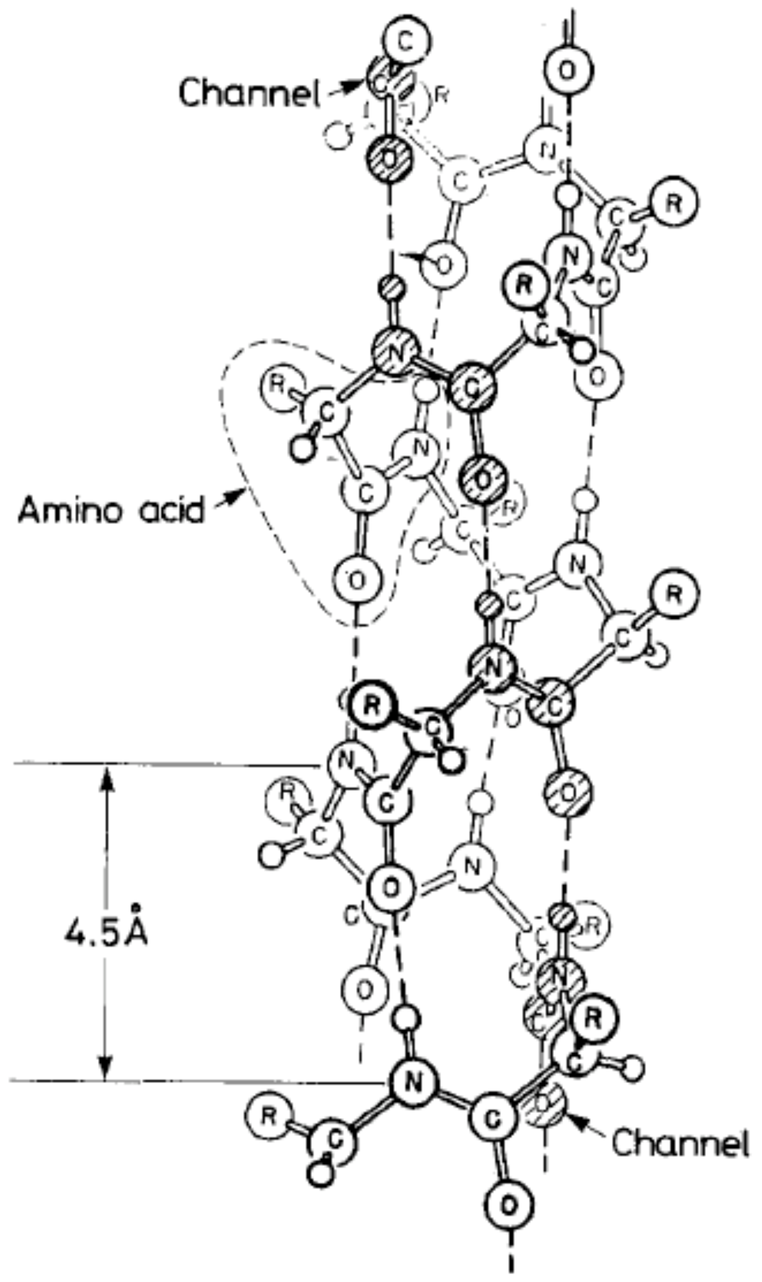
Holstein polaron and solitons in biomolecules

$$i\gamma\frac{dC_n}{d\tau} = -\left(\sum_{\delta[n]} C_{n+\delta}\right) + kC_n u_n\,,$$

$$\frac{d^2u_n}{d\tau^2} + u_n + k|C_n|^2 = 0.$$

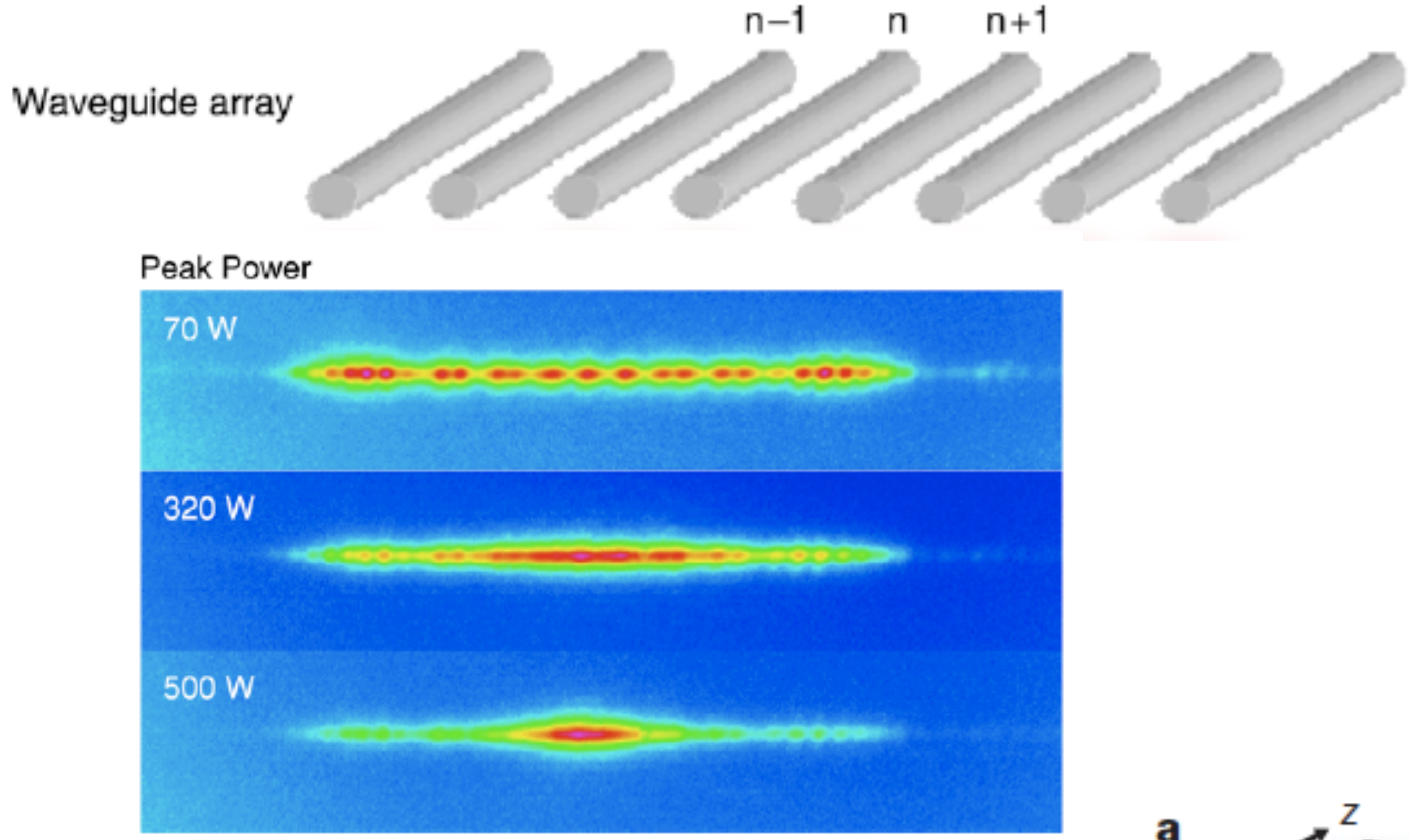


Kalosakas et al (1999)



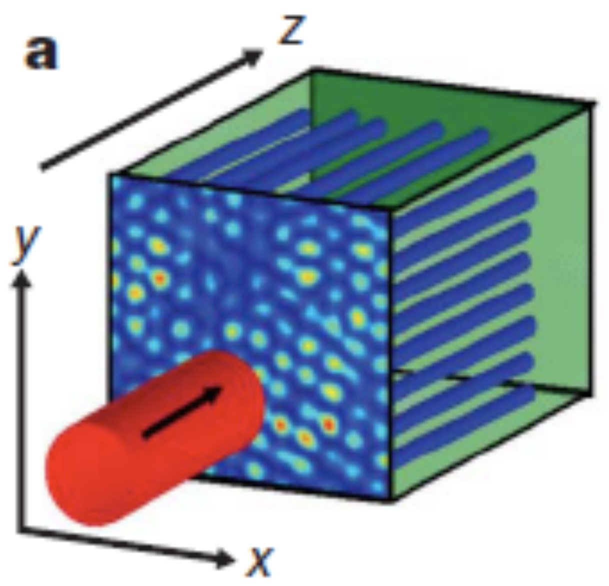
Scott (1992)

Optical fibers and DNLS

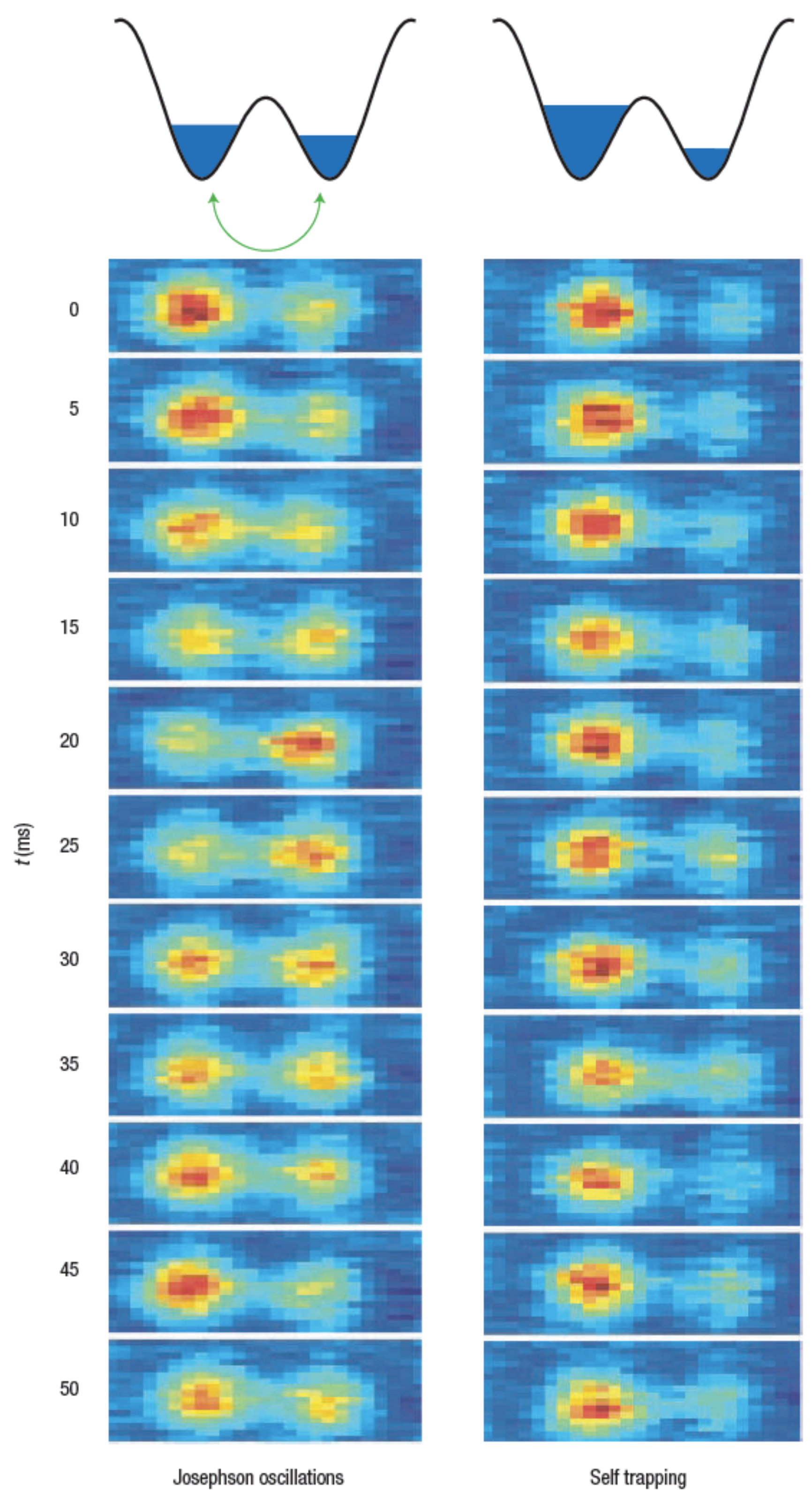


Eisenberg et al (2000)

Schwartz et al (2007)

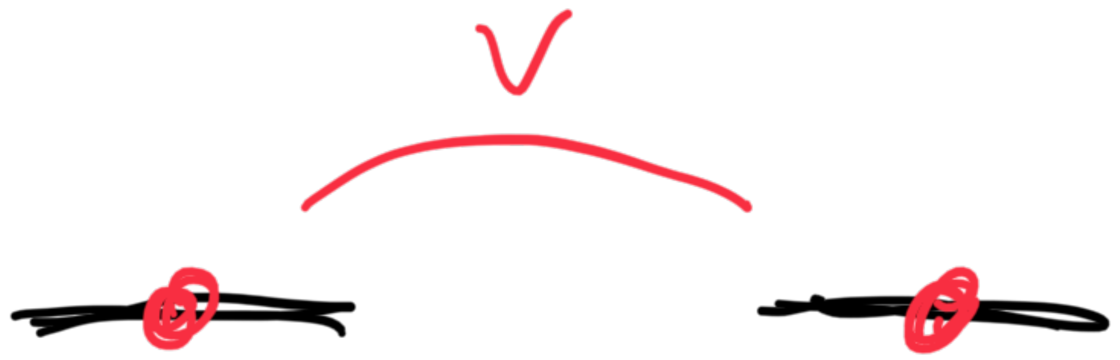


BEC



Bloch (2005)

The nonlinear dimer



$$i\dot{\psi}_1 = V\psi_2 - \chi|\psi_1|^2\psi_1$$

$$i\dot{\psi}_2 = V\psi_1 - \chi|\psi_2|^2\psi_2$$

Integrable in terms of elliptic functions

Seltrapping transition

RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 34, NUMBER 7 1 OCTOBER 1986

Self-trapping on a dimer: Time-dependent solutions of a discrete nonlinear Schrödinger equation

V. M. Kenkre
Department of Physics and Astronomy, University of New Mexico, Albuquerque, New Mexico 87131

D. K. Campbell
Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 19 May 1986)

From the discrete nonlinear Schrödinger equation describing transport on a dimer we derive and solve a closed nonlinear equation for the site-occupation probability difference. Our results, which are directly relevant to specific experiments such as neutron scattering in physically realizable dimers, exhibit a transition from "free" to "self-trapped" behavior and illustrate features expected in extended systems, including soliton/polaron bandwidth reduction and the dependence of energy-transfer efficiency on initial conditions.

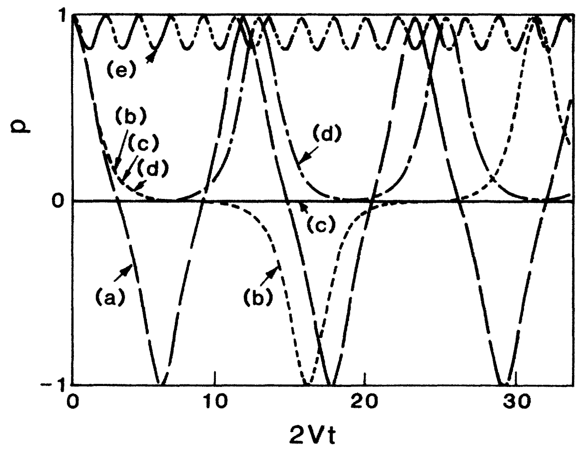


FIG. 1. The difference in the probabilities of occupation of the two sites in a dimer plotted as a function of time t for various values of $(\chi/4V)$: (a) 0.95, (b) 0.9995, (c) 1, (d) 1.0001, (e) 1.75. Curves (a) and (b) are indicative of free particle motion, (c) describes the transition, and (d) and (e) represent self-trapping behavior [see Eqs. (6) and (7)].

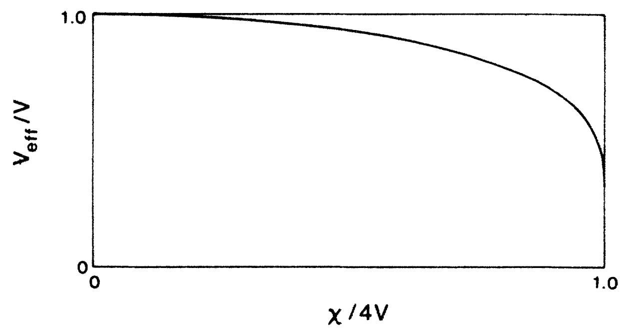


FIG. 2. The ratio of the effective bandwidth for motion between the dimer sites to the bare bandwidth plotted as a function of $(\chi/4V)$ showing a logarithmic reduction near the transition [see Eq. (11)].

INITIAL CONDITION EFFECTS IN THE EVOLUTION OF A NONLINEAR DIMER ☆

G.P. TSIRONIS [1] and V.M. KENKRE
Department of Physics and Astronomy, University of New Mexico, Albuquerque, NM 87131, USA

Received 11 July 1987, revised manuscript received 9 December 1987, accepted for publication 14 December 1987
Communicated by A.R Bishop

The initial state analysis of the evolution of a nonlinear degenerate dimer shows that, in addition to the self-trapping transition, a new transition occurs while the particle is in the trapped region. This transition can be understood in part in terms of the behavior of a linear nondegenerate dimer, and is intimately related to the stationary states of the nonlinear dimer

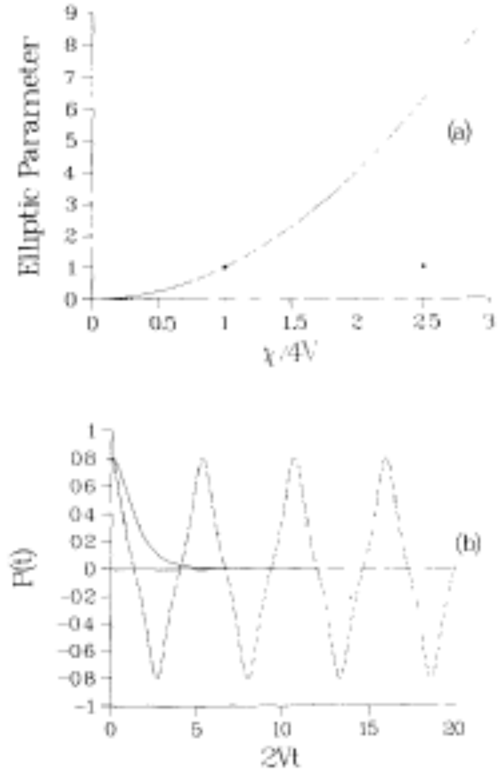


Fig 1 $r_0>0$ In (a) the elliptic parameter k^2 is plotted as a function of $k_0=\chi/4V$ for $p_0=1$ (full line) and 0 8 (dotted line) The bullet (●) shows the position of the self-trapping transition In (b) the time evolution of the probability difference $p(t)$ is plotted as a function of the time for $p_0=0$ 8 and for different values of k_0, 2 3 (dashed line), 2 5 (full line) and 2 7 (dotted line)

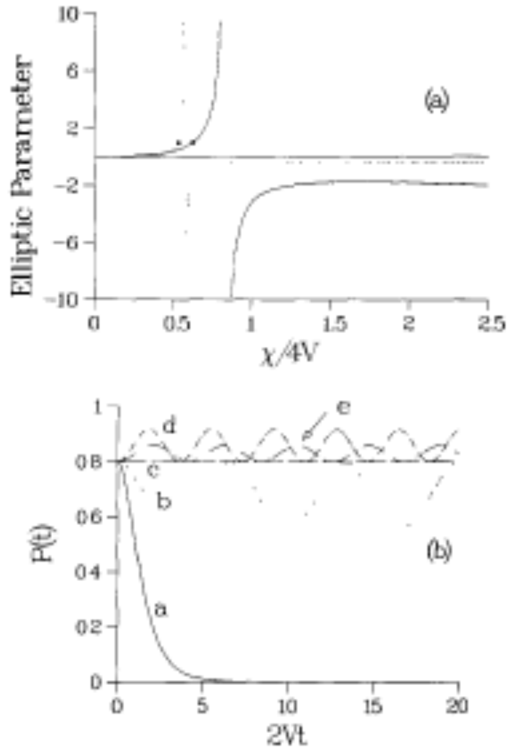
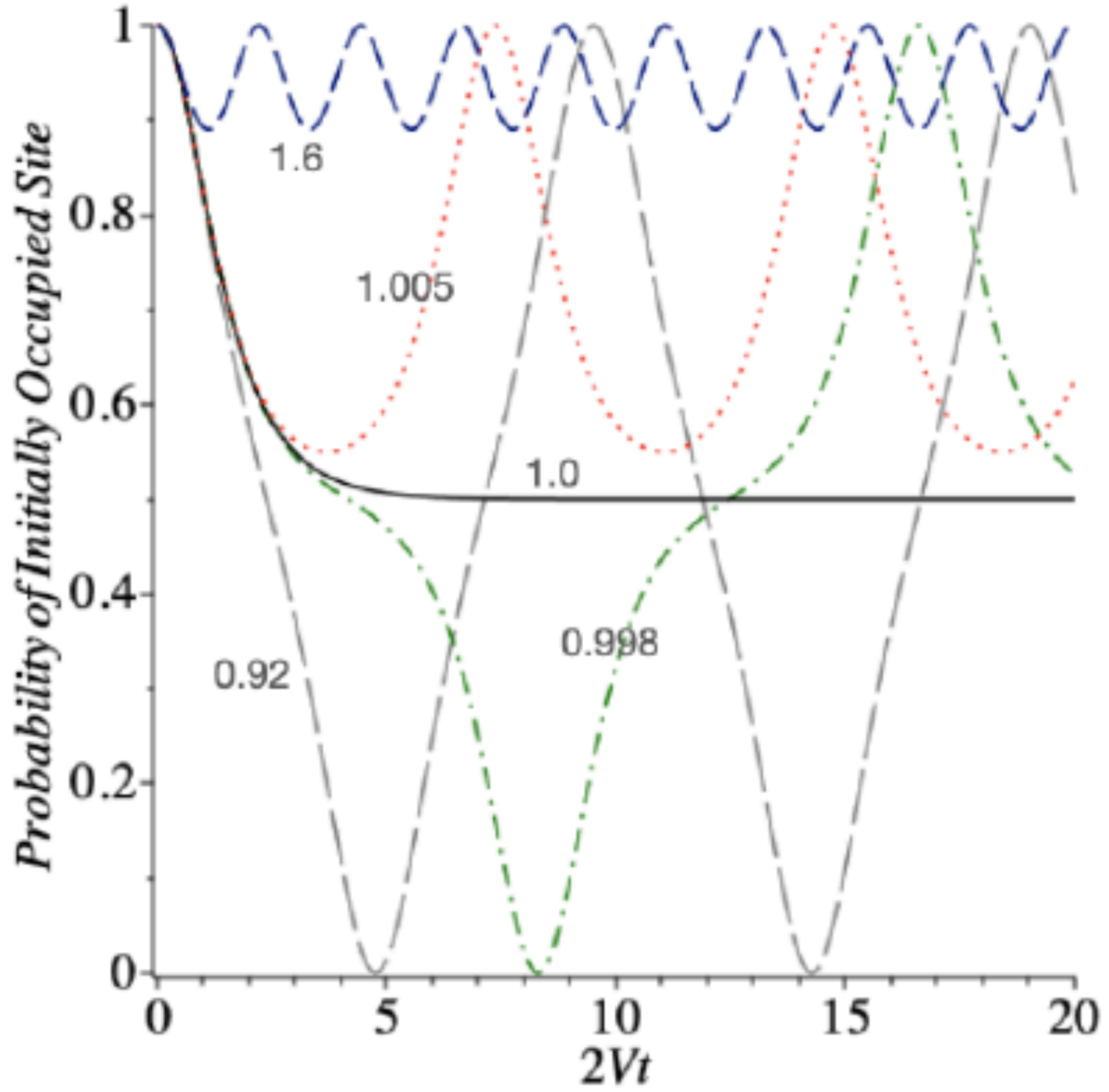
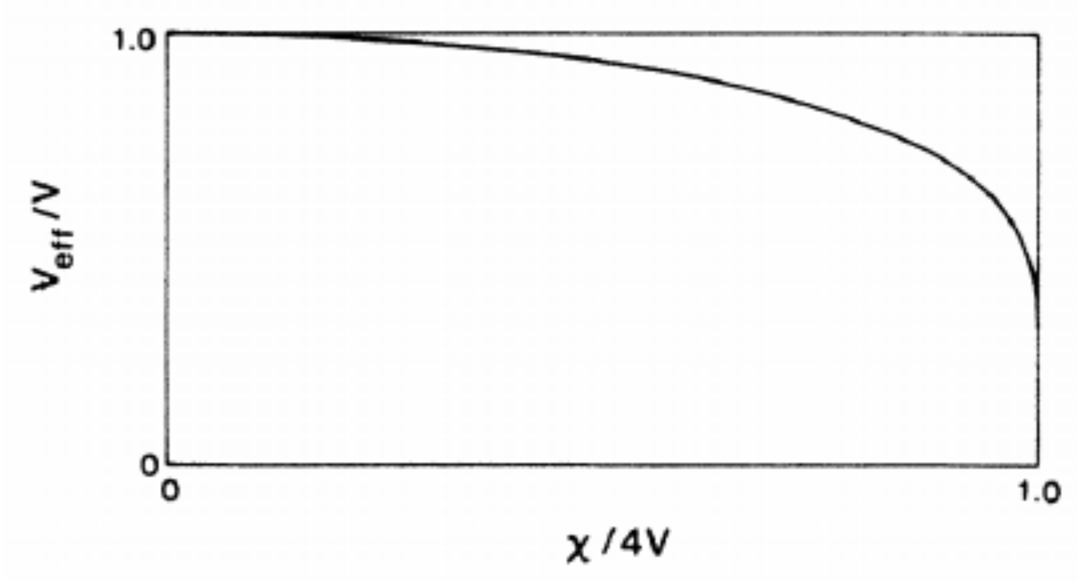


Fig 2 $r_0<0$: In (a) the elliptic parameter k^2 is plotted as a function of $k_0=\chi/4V$ for $p_0=0.8$ (full line) and 0 5 (dashed line). The bullet (●) shows when the self-trapping transition occurs In (b) $p_0=0.8$ and the values of k_0 are: (a) 0 625, self-trapping transition, (b) 0.7, the particle is trapped (dn-evolution), (c) 0 833, amplitude transition; the system occupies the stable stationary state, (d) 0 9 and (e) 1.0 (trapped-nd)



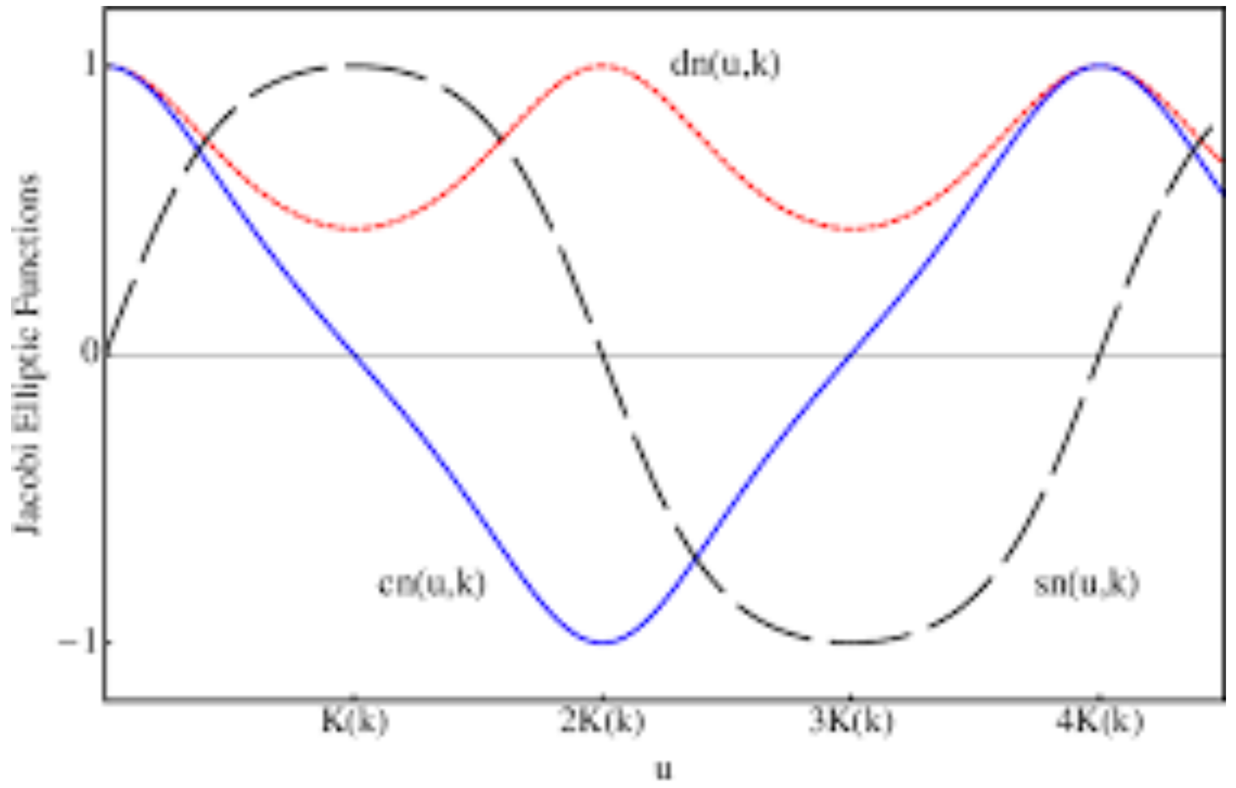


$$T = \frac{2K(k)}{V} = \frac{2}{V}\int_0^1 \frac{dz}{\sqrt{1-z^2}\sqrt{1-k^2z^2}}.$$

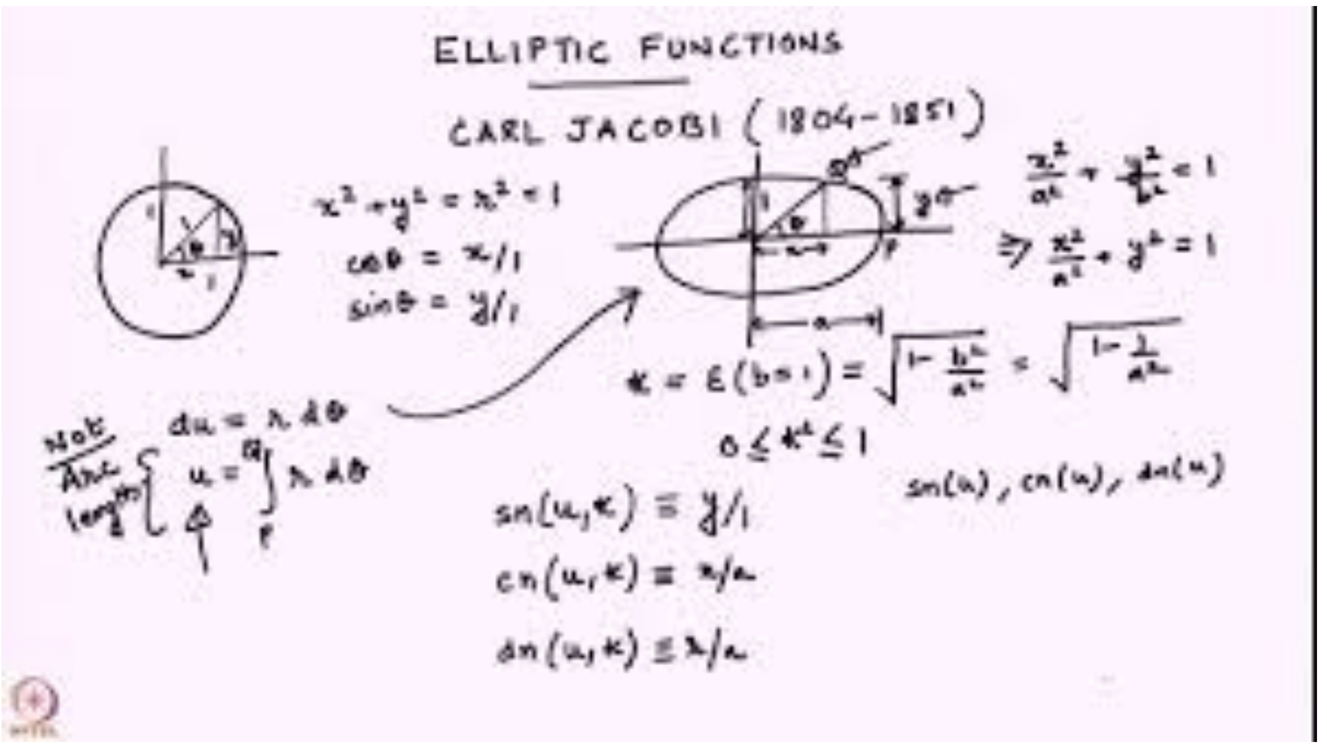
$$p(t) = \mathrm{cn}\left(2Vt, \frac{\chi}{4V}\right) \quad \text{for } \chi \leq 4V.$$

$$p(t) = \mathrm{dn}\left(\frac{\chi t}{2}, \frac{4V}{\chi}\right) \quad \text{for } \chi \geq 4V.$$

Jacobian elliptic functions



$$u = \int_0^{\phi} \frac{dt}{\sqrt{1 - k^2 \sin^2 t}}$$



$\mathrm{cd}(z \mid 0) = \cos(z)$	$\mathrm{cd}\left(z + \frac{\pi}{2} \middle\vert 0\right) = -\sin(z)$	$\mathrm{cd}(z \mid 1) = 1$
$\mathrm{cn}(z \mid 0) = \cos(z)$	$\mathrm{cn}\left(z + \frac{\pi}{2} \middle\vert 0\right) = -\sin(z)$	$\mathrm{cn}(z \mid 1) = \mathrm{sech}(z)$
$\mathrm{cs}(z \mid 0) = \cot(z)$	$\mathrm{cs}\left(z + \frac{\pi}{2} \middle\vert 0\right) = -\tan(z)$	$\mathrm{cs}(z \mid 1) = \mathrm{csch}(z)$
$\mathrm{dc}(z \mid 0) = \sec(z)$	$\mathrm{dc}\left(z + \frac{\pi}{2} \middle\vert 0\right) = -\csc(z)$	$\mathrm{dc}(z \mid 1) = 1$
$\mathrm{dn}(z \mid 0) = 1$	$\mathrm{dn}(z \mid 1) = \mathrm{sech}(z)$	$\mathrm{dn}\left(z + \frac{\pi i}{2} \middle\vert 1\right) = -i\,\mathrm{csch}(z)$
$\mathrm{ds}(z \mid 0) = \csc(z)$	$\mathrm{ds}\left(z + \frac{\pi}{2} \middle\vert 0\right) = \sec(z)$	$\mathrm{ds}\left(z + \frac{\pi i}{2} \middle\vert 1\right) = -i\,\mathrm{sech}(z)$
$\mathrm{nc}(z \mid 0) = \sec(z)$	$\mathrm{nc}\left(z + \frac{\pi}{2} \middle\vert 0\right) = -\csc(z)$	$\mathrm{nc}(z \mid 1) = \cosh(z)$
$\mathrm{nd}(z \mid 0) = 1$	$\mathrm{nd}(z \mid 1) = \cosh(z)$	$\mathrm{nd}\left(z + \frac{\pi i}{2} \middle\vert 1\right) = i \sinh(z)$
$\mathrm{ns}(z \mid 0) = \csc(z)$	$\mathrm{ns}\left(z + \frac{\pi}{2} \middle\vert 0\right) = \sec(z)$	$\mathrm{ns}(z \mid 1) = \coth(z)$
$\mathrm{sc}(z \mid 0) = \tan(z)$	$\mathrm{sc}\left(z + \frac{\pi}{2} \middle\vert 0\right) = -\cot(z)$	$\mathrm{sc}(z \mid 1) = \sinh(z)$
$\mathrm{sd}(z \mid 0) = \sin(z)$	$\mathrm{sd}\left(z + \frac{\pi}{2} \middle\vert 0\right) = \cos(z)$	$\mathrm{sd}(z \mid 1) = \sinh(z)$
$\mathrm{sn}(z \mid 0) = \sin(z)$	$\mathrm{sn}\left(z + \frac{\pi}{2} \middle\vert 0\right) = \cos(z)$	$\mathrm{sn}(z \mid 1) = \tanh(z).$

$$\mathrm{sn}(u) = \frac{2\pi}{K\sqrt{m}} \sum_{n=0}^{\infty} \frac{q^{n+1/2}}{1 - q^{2n+1}} \sin((2n+1)v)$$

$$\mathrm{cn}(u) = \frac{2\pi}{K\sqrt{m}} \sum_{n=0}^{\infty} \frac{q^{n+1/2}}{1 + q^{2n+1}} \cos((2n+1)v)$$

$$\mathrm{dn}(u) = \frac{\pi}{2K} + \frac{2\pi}{K} \sum_{n=1}^{\infty} \frac{q^{n}}{1 + q^{2n}} \cos(2nv).$$