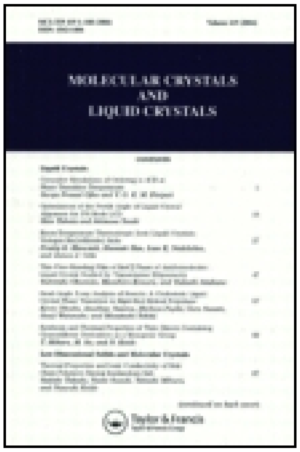

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Time Variation of Energy in Colliding Solitons in Polyacetylene

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TIME VARIATION OF ENERGY IN COLLIDING SOLITONS IN POLYACETYLENE

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Abstract Time variation of energy and number of solitons in colliding process are examined in polyacetylene. It is strongly dependent on the soliton velocity, but weakly on the soliton width.

THEORY

From the canonical transformation of SSH Hamiltonian we have the electronic part H_S as

$$H_s = \sum_{k}(B+ Ak^2)a^+_k a_k - \frac{F}{2N}\sum_{k_1 - k_3} a^+_{k_3-k_1} a^+_{k_2} a_{k_3} a_{k_2-k_1} \qquad (1)$$

In the coherent state representation the two-soliton function is given by $\alpha_1(x,t)+\alpha_2(x,t)$ where[1]

$$\alpha(x,t)=\sqrt{\zeta}\,\mathrm{sech}\left[2\zeta(x- x_0-4c\tau)\right]\exp i\left[2cx- 4(c^2-\zeta^2)\tau+\theta\right], \qquad (2)$$

$\tau = At/\hbar$ and the total energy as

$$\begin{aligned} E &= \langle\alpha_1+\alpha_2|H_s|\alpha_1+\alpha_2\rangle \\ &= \frac{Nd}{2\pi}\int dq\, n_q(B+ Aq^2) - \frac{F}{2d}\int dx\, |\alpha_1(x,t) +\alpha_2(x,t)|^4 \qquad (3) \\ &= BN_s + AN_k - \frac{F}{4d\xi}\cdot SSC \text{ or } SAC, \quad \xi = 1/(2\zeta) \end{aligned}$$

where N_s, N_k and SSC(SAC) correspond to soliton number, kinetic and correlation energies. Two solitons are located at $x= \pm x_0$ at $\tau=0$, and collide at $\tau_0(=x_0/4c)$. $c_1= -c_2= c$. We consider two kinds of pair; soliton-soliton(SS), and soliton-antisoliton(SA). Correspondingly we put $N_s=$ SSN or SAN, $N_k=$ SSQ or SAQ in Figures.

RESULT AND DISCUSSION

By numerical computation we examined the constancy of energy and number of solitons in course of time $0\to\tau_0$. The behaviors of static (number), kinetic and correlation energies are shown in Table I and Figures 1 3. It is found that the time variation is strongly dependent on AL(= $2c\xi \sim$ soliton velocity$\times$width), and small for large AL, but remarkable for small AL. Also it is very weakly dependent on GD(=$\xi/d \sim$ soliton width).

The reason that the constancy of energy does not hold will be because $|\alpha_1 + \alpha_2\rangle$ is not an exact eigenfunction of H_s. The employed parameters are not exact enough, which may cause some computational error. Also the separation of electronic and lattice parts is not exact quantum-mechanically, being of the order of square of electron phonon coupling through which the surplus or defficient energy is transferred to and from the lattice.

The large soliton velocity means the small electron-phonon coupling. In this case the soliton is almost an exciton which runs scattering phonons. Contrary, the small soliton velocity means the large electron phonon coupling. In this case the soliton is almost a trapped polariton. Some authors[2,3] have estimated the soliton velocity in polyacetylene as $v_{sol} \lesssim 2.6 v_{sound}$ and $v_{sound} = 1.85 \times 10^6$ cm/s. So, we take $v_{sol} = 2.0 v_{sound}$, then we have AL= 1.06(GD= 7), 0.75(GD= 5) which lie in the region of our assumption; AL= 3, 1, 0.5. By the scheme of Ruckh et al[4] they have $v_{sol} < v_{sound}$. This is the strong coupling case.

Table I. Variations of total energy E and soliton number N_s with time. E in 2.50 eV. N_s= 2.0 at = 0.

		E(SS)		N_s	E(SA)		N_s
AL	GD	τ/τ_0= 0	0.9	1.0	0	0.9	1.0
3	3	6.010	5.933	2.00	6.010	5.933	2.00
	5	5.344	5.273	2.00	5.344	5.270	2.00
	7	5.166	5.109	2.00	5.166	5.103	2.00
1	3	5.050	5.573	2.54	5.050	4.370	1.55
	5	4.999	5.892	2.54	4.980	3.954	1.55
	7	4.988	6.045	2.54	4.992	3.809	1.55
0.5	3	4.960	6.911	3.37	4.960	2.821	0.63
	5	4.964	7.612	3.37	4.969	2.138	0.63
	7	4.978	7.897	3.37	4.968	1.899	0.63

Fig. 1 SOLITON NUMBER

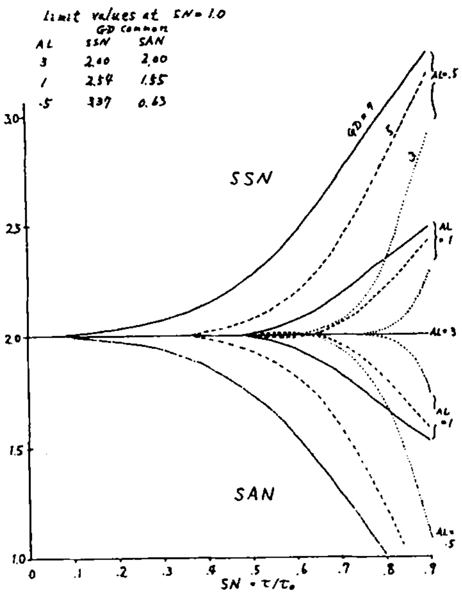
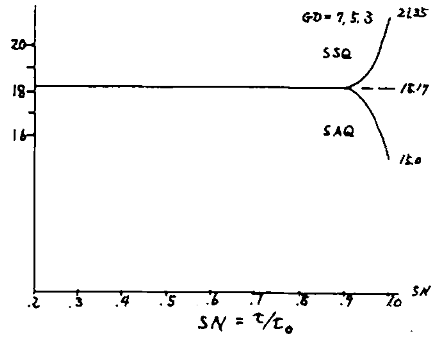
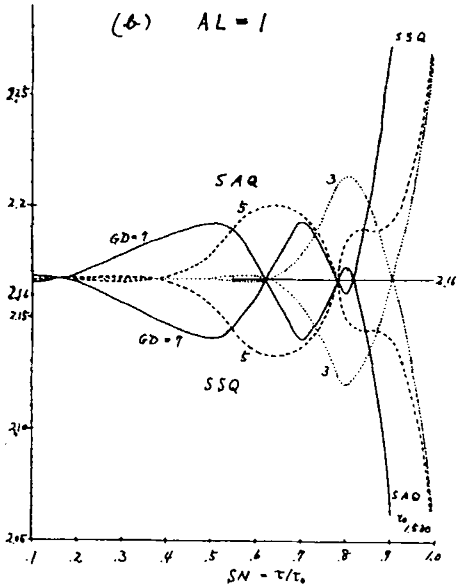


Fig. 2 KINETIC ENERGY

(a) AL = 3



(b) AL = 1



(c) AL = 0.5

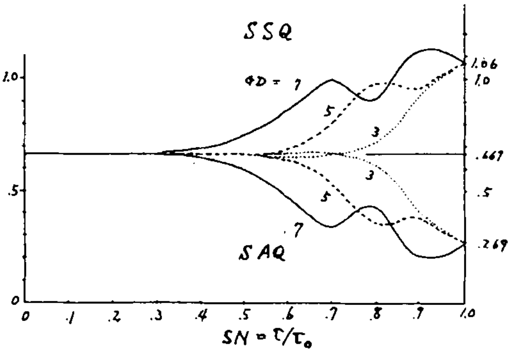
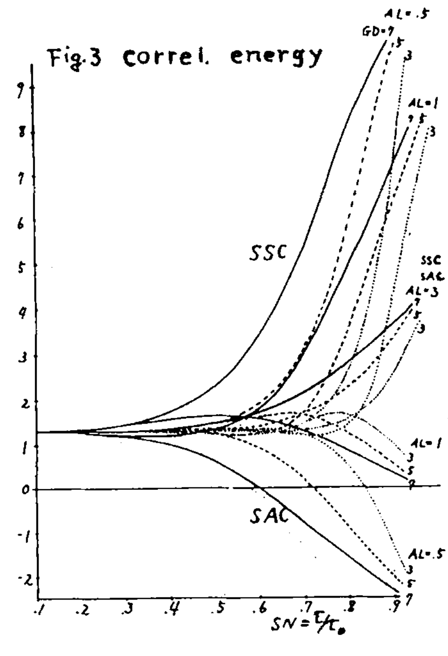


Fig. 3 correl. energy



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