の相対的な滑りによっておこる筋収縮は，この力によって起されていると考えられる．この過程で行われる力学的仕事によってソリトンのエネルギーと振幅はゼロになるまで，そしてソリトンの速度は $v_0 \simeq 4.5 \times 10^5$ cm/sec になるまで減少する．最初につくられるソリトンを特徴づけている κ の最大値はソリトンのエネルギーをＡＴＰの加水分解で解放されるエネルギー 0.49 eVに等しいとおいて近似的に評価される；$\kappa \simeq 2.9$．格子収縮或はこれに相当する格子張力のソリトンの最大振幅は

$$|r/D|_{\max} = 0.12, \quad f_{\max} = 2.0 \times 10^{-4}\,\text{dyne} \tag{7}$$

と評価され，ソリトン波の幅は $2D/\kappa = 3.2$ Å と評価される．これらは驚くべき合理的な値を与えている．筋肉が1kg重（10^6dyne）の程度の力を出すために同時に働かなければならないミオシン分子の数は(7)の $f_{\max}$ の値から約 $N \simeq 10^6/10^{-4} = 10^{10}$ と推定される．一方，脊椎動物の横紋筋は約100万の筋繊維からなる組織であり，各筋繊維は同様なサルコメアからなる約千のミオフィブリルを含んでおり，サルコメアの中心は約2～3百のミオシン分子を含む太いフィラメントで占められている．結局，一つの横紋筋は約 10^{11} 個のミオシン分子を含んでいる．従って，上に述べた理論的な評価は横紋筋の中にあるミオシン分子の数について合理的な数を与えている．ミオシン分子の頭が行うひっかき運動(scratching motion)の時間は（ミオシンヘッド或はクロスブリッジの長さ）/（ソリトンの速さ）$\simeq 250$ Å $/ 4.5 \times 10^5$ cm/s $\simeq 6$ picosecond の程度と推定される．picosecond の程度の周期をもったミオシンの頭の運動を検出する実験が切望される．

Polypeptide系と分子性結晶におけるvibron soliton

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1. INTRODUCTION

A characteristic feature which exists in biologically important macromolecules such as proteins and DNA is their structural and dynamical flexibility. This reflects the fact that many functional properties of these molecules cannot be completely understood from the average structure as determined by x-ray analysis. For example, reaction rates of enzymes may be correlated with the structural and dynamical flexibility of proteins, while local structural fluctuations in DNA may be a part of what proteins recognize. As is well known, recent development of nonlinear science has yielded new and interdisciplinary concepts such as solitons, universal routes to chaos, fractals, pattern selection and so

on. Of these soliton problem has produced a unifying influence in natural science. The aim of this paper is to explore the utility of soliton concept in understanding the structural and dynamical properties of proteins.

2. MODEL DYNAMICAL SYSTEM

To simulate proteins, we consider a 1d oscillator system, in which each oscillator is linearly coupled with neighbouring ones and nonlinearly with lattice vibrations. The oscillator Hamiltonian H_{osc} is given by

$$H_{osc}=\sum_n[(m\dot{q}_n^2/2)+v(q_n)]-\sum_{nn'}L(n,n')q_nq_{n'},\quad L(n,n')=L(|n-n'|). \tag{2.1}$$

Here q_n, $v(q_n)$, and $L(n,n')$ are the normal coordinate of the nth oscillator with effective mass m, an on-site potential, and a force constant, respectively. Two types of lattice vibrations are considered, acoustic and optic vibrations, the former and the latter being given by the Hamiltonian

$$H_{La}=\sum_n[(M\dot{u}_n^2/2)+K(u_{n+1}-u_n)^2] \quad \text{with} \quad H'_{La}=\sum_n[V(q_n)(u_{n+1}-u_{n-1})] \tag{2.2}$$

and

$$H_{Lo}=\sum_n[(M\dot{u}_n^2/2)+Ku_n^2] \quad \text{with} \quad H'_{Lo}=\sum_n V(q_n)u_n, \tag{2.3},$$

respectively. Here u_n and K are the displacement of the nth molecule with molecular mass M from its equilibrium position and a force constant respectively. Oscillator-lattice interactions are described by the Hamiltonian H'_{La} or H'_{Lo} in which $V(q_n)$ is a function of q_n^2. For these two model systems equations of motion for the q_n's and the u_n' take the form

(i) case of acoustic phonons

$$m\ddot{q}_n+v'(q_n)-2\sum_{n'}L(n,n')q_{n'}+V'(q_n)(u_{n+1}-u_{n-1})=0, \tag{2.4a}$$

$$M\ddot{u}_n+K(u_{n+1}+u_{n-1}-2u_n)-[V(q_{n+1})-V(q_{n-1})]=0, \tag{2.4b}$$

(ii) case of optic phonons

$$m\ddot{q}_n+v'(q_n)-2\sum_{n'}L(n,n')q_{n'}+V'(q_n)u_n=0, \tag{2.5a}$$

$$M\ddot{u}_n+Ku_n+V(q_n)=0. \tag{2.5b}$$

If the velocity v of nonlinear excitations under consideration is much smaller than the velocity of phonons in case (i) and it satisfies the relation $Mv^2\ll Ku^2$ in case (ii), the factor $M\ddot{u}_n$ can be neglected to give

$$u_{n+1}-u_n=-(1/K)[V(q_{n+1})+V(q_n)]+(u_0/2) \qquad \text{for case (i)} \tag{2.6}$$

$$u_n=-V(q_n)/K \qquad \text{for case (ii)} \tag{2.7}$$

where u_0 is an integral constant. It is understood that the u_n's here depend only on the secular part $V(|Q_n|^2)$ of $V(q_n)=V(q_n^2)$, where Q_n and Q_n^* are the negative and position frequency parts of q_n, respectively. Inserting Eqs.(2.6) and (2.7) back into Eqs.(2.4a) and (2.5a), respectively, we get equations of motion written entirely in terms of the q's derivable from the following effective oscillator Hamiltonian

$$H_{eff}=\sum_n[(m\dot{q}_n^2/2)+U(q_n)]-\sum_{nn'}L(n,n')q_nq_{n'}+\sum_n W(q_n,q_{n+1}) \tag{2.8}$$

where

$$U(q_n)=\begin{cases} v(q_n)+u_0V(q_n)-(2/K)V(q_n)^2 & \text{for case (i)} \quad (2.9a) \\ v(q_n)-(1/2K)V(q_n)^2 & \text{for case (ii)} \quad (2.9b) \end{cases}$$

$$W(q_n,q_{n+1})=\begin{cases} -(1/K)V(q_n)[V(q_{n+1}-V(q_n)] & \text{for case (i)} \quad (2.10a) \\ 0 & \text{for case (ii)} \quad (2.10b) \end{cases}$$

The on-site potential v(q) is modified into the effective one U(q) by the oscillator-lattice interactions, where nonlinear attractive potentials characterized by the factor $-V(q)^2/K$ are induced. Two more effects exist for case (i). Namely, $u_0V(q_n)$ and $W(q_n,q_{n+1})$ represent a modification of $v(q_n)$ due to the existence of strain field and phonon-assisted vibration transfer, respectively. In a sense, the result so obtained for low velocity nonlinear excitations, which appear to play a crucial role in nonlinear phenomena in biological systems, can be considered as arising from a coherent part of the oscillator-lattice interactions.

3. DYNAMICAL SELF TRAPPING OF VIBRONS

To study the effect of the nonlinear attractive potential, we put $u_0=0$ and neglect phonon-assisted vibration transfer for case (i). As the simplest yet most important model, we take

$$v(q)=m\omega_0^2q^2/2, \qquad V(q)=Aq^2/2. \quad (3.1)$$

Here ω_0 and A are an eigenfrequency of the oscillator and a coupling constant, respectively. An explicit expression for the effective on-site potential U(q) is then obtained as follows

$$U(q)=\begin{cases} (m\omega_0^2/2)q^2-(A^2/2K)q^4 & \text{for case (i)} \quad (3.2a) \\ (m\omega_0^2/2)q^2-(A^2/8K)q^4 & \text{for case (ii)} \quad (3.2b) \end{cases}$$

We are particularly interested in localized modes induced by the nonlinear attractive potential appearing below the bottom $\omega_1=\omega^{(0)}(0)$ of the vibron frequency band $\omega^{(0)}(k)=[\omega_0^2-(2/m)\sum_n L(n)\exp(ikna)]^{1/2}$ as shown in Fig.1. Here a is the lattice constant of the oscillator system This is a self-trapped state of vibrons referred to as vibron solitons. Here we limit our discussion to case (ii), since Eqs.(3.2a) and (3.2b) are of the same form, and such solitons has been identified in red-shifted infrared spectra of amide I vibrons in crystalline acetanilide or ACN $(CH_3CONHC_6H_5)_x$ recognized as a quasi-polypeptide system.[1] In studying equations of motion for the q's governed by Eq.(2.8) with U(q) given by Eq.(3.2b), we put $q_n=Q_n+Q_n^*$ with $Q_n\simeq\exp(-i\omega_1t)$ and employ the rotating-wave approximation to obtain

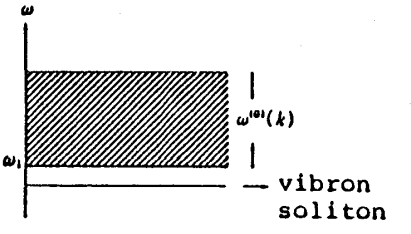

Fig.1

$$\ddot{Q}_n+\omega_0^2Q_n-(2/m)\sum_{n'}L(n,n')Q_{n'}-(3A^2/2Km)|Q_n|^2Q_n=0 \quad (3.3)$$

with

$$u_n=-(A/K)|Q_n|^2. \quad (3.4)$$

We seek solutions to this in the form $Q_n=f_n\exp[-i(\omega t-kna)]$, where k and

ω are real constants identified as the momentum and eigenfrequency of vibron solitons, respectively, while f_n is a real envelope function. Inserting this into Eq.(3.3) gives

$$\ddot{f}_n+[\omega^{(0)}(k)^2-\omega^2]f_n-(2L/m)\cos(ka)(f_{n+1}+f_{n-1}-2f_n)-(3A^2/2Km)f_n^3=0 \quad (3.5a)$$

$$2\omega\dot{f}_n+(2L/m)\sin(ka)(f_{n+1}-f_{n-1})=0. \quad (3.5b)$$

Here we employed a nearest neighbour approximation for L(n,n') with L=L(1). Except in the case of a continuum limit, where solutions to Eq.(3.5) have a form similar to those to the 1d nonlinear Schrödinger equation, the above equations cannot be solved analytically.

Let us pay attention to stationary localized modes for which k=0 and f_n is time-independent. A red-shifted absorption band at about 1650 cm^{-1} in ACN as shown in Fig.2 can be considered as being due to such solitons.[1] Equation (3.5a) then reduces to

$$\omega_0^2 f_n-(2L/m)(f_{n+1}+f_{n-1})-(3A^2/2Km)f_n^3=\omega^2 f_n, \quad (3.6)$$

while (3.5b) is automatically satisfied. In terms 1d lattice Green's functions

$$G(n,n';\omega)=\frac{1}{N}\sum_k \frac{\exp[ik(n-n')a]}{\omega^{(0)}(k)^2-\omega^2} \quad (3.7)$$

and the soliton amplitude b defined by $f_n=bw_n$ with max $|w_n|=1$, Eq.(3.7) is rewritten as

$$w_n=(3A^2b^2/2Km)\sum_{n'} G(n,n';\omega)w_{n'}^3, \quad (3.8)$$

This is treated by using a successive approximation. We pay particular attention to a spatially symmetric or s-like mode $w_n=w_{-n}$ localized at n=0. Here the assessment of the localization of the localized mode is required by estimating numerical values of L, m, A and K, in addition to the amide I frequency $\omega_0=1665\ cm^{-1}$. Making one-to-one correspondence to the theory in ref.[1] based on the Davydov theory,[2] we get

$$J=\hbar L/m\omega_0=3\sim 4\ cm^{-1},\ K=1.3\times 10\ N/m,$$

$$\chi=\hbar A/2m\omega_0=6\times 10^{-11}\ N,\ \hbar\omega_1=1665\ cm^{-1}$$

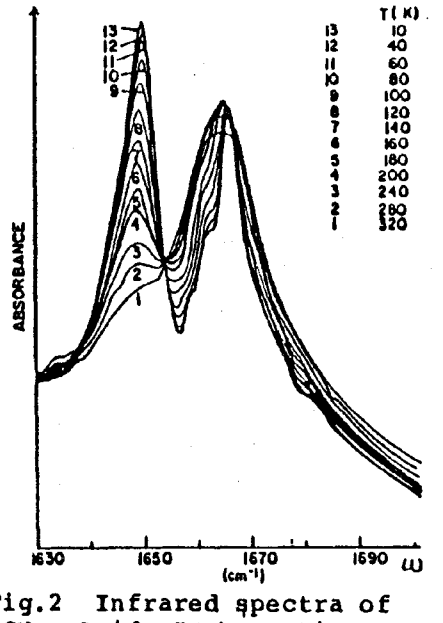

Fig.2 Infrared spectra of ACN. Amide I absorption at 1665 cm^{-1} is red-shifted to 1650 cm^{-1}. (data by Care et al ref[1])

In terms of $\epsilon=\hbar(\omega_1-\omega)/2J$ and $y=(m\omega_0/\hbar)b^2$, the lattice Green's function $G(n,n';\omega)=G(n-n;\omega)$ is written as

$$G(n;\omega)=By[(1+\epsilon)^2-1]^{-1/2}\{1+\epsilon+[(1+\epsilon)^2-1]^{1/2}\}^{-|n|}, \quad (3.9)$$

where

$$B=(3/2)(\chi^2/KJ)=7.5 \text{ for } J=3\ cm^{-1} \text{ and } 5.6 \text{ for } J=4\ cm^{-1}. \quad (3.10)$$

The yet undetermined factor y is taken to be 1/2. This corresponds to the soliton amplitude associated with the zero-point motion of the amide I vibration. As the first order approximation, we assume that the localized mode is strongly localized at the site n=0. Equation (3.8) then

reduces to

$$1 - (3A^2b^2/2Km)G(0;\omega)=0 \quad \text{or} \quad \epsilon=(B^2y^2+1)^{1/2}-1. \tag{3.11}$$

Inserting the numerical values obtained above to this, we get ϵ =2.9 for J=3 cm^{-1} and 2.0 for J=4 cm^{-1}. The binding energy $E_B=\hbar(\omega_1-\omega)$ of solitons, which corresponds to a red-shift frequency of amide I absorption line in ACN, is E_B=17.4 cm^{-1} for J=3 cm^{-1} and 16.0 cm^{-1} for J=4 cm^{-1}. The quantity $\{1+\epsilon+[(1+\epsilon)^2-1]^{1/2}\}^{-1}$, which is a measure of the localization of the vibron solitons, is 0.13 and 0.17 for these two values of J. This implies that our first order approximation is actually a good approximation, and we do not need to proceed any more. The soliton binding energy so obtained is good agreement with the experimental result obtained by Careri et al.[1] Here we have not yet specified optical phonons with which the amide I vibration in ACN couples. These may be phonon modes involving proton motion. It is seen from Eq.(3.4) that a local strain field or coherent phonon field is accompanied with stationary vibron solitons.

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K－dV方程式の一般的座標変換

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ソリトン方程式と呼ばれる方程式の中には適当な変換によって結びつけられるものがある．その一例として，Konno-Ichikawa-Wadati方程式[1]

$$\theta_\tau + \cos^2\theta\,(\sin\theta)_{\xi\xi\xi} = 0 \tag{1}$$

は，Ishimori[2]によって見付けられた変換

$$\begin{cases} \xi = \int^x \cos\theta\, dx \\ \tau = t \end{cases} \tag{2}$$

によって次のようなmodified K-dV方程式

$$\theta_t + \frac{1}{2}\theta_x^3 + \theta_{xxx} = 0 \tag{3}$$