Vibrational modes around the soliton in strongly coupled one-dimensional electron-lattice systems

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The vibrational properties of strongly coupled one-dimensional electron-lattice systems are distinct from those of weakly coupled ones. While the weakly coupled systems have only four localized modes around the soliton and there is overlap between acoustic and optical phonon branches, the strongly coupled system can possess more localized modes, and no overlap exists. In terms of the coupling constant λ, the boundary between strong and weak coupling is $\lambda_c = 0.2119$. The number of localized modes depends on λ, and each localized mode can only exist for a certain region of λ. Then the whole range $[0,2/\pi]$ of λ can be divided into seven regions, each of which has a characteristic disposition of the localized modes.

The nonlinear excitations in one-dimensional (1D) electron-lattice coupled systems, such as solitons and polarons, greatly influence the dynamic processes. One important aspect is the localized modes around the soliton and polaron. In recent years much attention has been focused on this subject. Starting from the Takayama, Lin-liu, and Maki (TLM) model,[1] which is the continuum version of the Su, Schrieffer, and Heeger (SSH) model[2] in the weak-coupling limit, Nakahara and Maki found two localized modes around the soliton by using a variational method,[3] i.e., the Goldstone mode g_1 and the amplitude mode g_2. Hicks and Blaisdell also got these two modes by a Green's-function technique.[4] Ito, Terai, Ono, and Wada established an integral eigenequation to determine the vibrational modes around nonlinear excitations, and they obtained one more localized mode g_3 around the soliton.[5] Sun and his co-workers pointed out that the TLM model might smear out some localized modes with rapidly varying configuration as a result of the continuum approximation, and, indeed, they found a new type of localized mode—the staggered mode g_s from the SSH model.[6] Terai and Ono,[7] Chao and Wang,[8] and Gammel[9] verified this mode independently. It should be noticed that all these results came out from weakly coupled situations, where the coupling constant $\lambda < 0.2$. However, the calculations made in Ref. 6 showed that another localized mode could emerge in the case of larger λ; the calculations indicate that the strongly coupled systems could possess some new vibrational modes, and the number of localized modes would depend on the coupling. Another factor affected by the strong coupling is the mobility of the soliton. When the coupling is weak, the width of the soliton is much larger than the lattice constant, the discreteness of the lattice can be neglected, and the soliton can slide freely. As the coupling gets stronger, the width of the soliton will become comparable to the lattice constant, and the mismatch between soliton and lattice will cause a barrier for soliton hopping. This paper studies the vibrational modes, especially the localized modes, around the soliton over the whole range of coupling strength. The criterion for a vibrational mode to be localized is to have the following behavior in the shape of its amplitude configuration: the wings of the configuration decay concavely, and when the length of the chain increases, the central part of the configuration does not expand and the wings approach zero. It should be mentioned that the resonance with the degenerate extended mode may make the wings of the localized modes go to a small finite oscillation.

The SSH Hamiltonian reads

$$H = -\sum_{n,s}[t_0 - \alpha(u_{n+1}-u_n)](a^\dagger_{n,s}a_{n+1,s} + \text{c.c.}) + \frac{K}{2}\sum_n (u_{n+1}-u_n)^2 + \frac{M}{2}\sum_n \dot{u}_n^2 , \quad (1)$$

all the notations have the conventional meaning. Introducing the dimensionless order parameter ϕ_n, the coupling constant λ, and the time τ as

$$\phi_n = (-1)^n \frac{\alpha}{t_0} u_n, \quad \lambda = \frac{2\alpha^2}{\pi t_0 K}, \quad \tau = \omega_Q t , \quad (2)$$

TABLE I. The regions and properties of localized modes.

Localized mode	Region of λ	Parity	Frequency ω/ω_Q
g_1	$0-2/\pi$	even	0
g_2	$0-2/\pi$	odd	$\lesssim 0.66$
g_3	0.13–0.41	even	0.55–0.71
g_4	0.22–0.43	odd	0.64–0.71
g_s	$0-2/\pi$	even	0.63–0.70
g'	0.276–0.284	odd	0.70

TABLE II. The dispositions of localized modes in seven regions of λ.

Region of λ	Disposition of localized modes
0–0.13	3 (g_1,g_2,g_s)
0.13–0.22	4 (g_1,g_2,g_3,g_s)
0.22–0.276	5 (g_1,g_2,g_s,g_3,g_4)
0.276–0.284	6 (g_1,g_2,g_s,g_3,g_4,g')
0.284–0.41	5 (g_1,g_2,g_s,g_3,g_4)
0.41–0.43	4 (g_1,g_2,g_s,g_3)
$0.43-2/\pi$	3 (g_1,g_2,g_s)

where $\omega_Q=(4K/M)^{1/2}$ is the bare frequency, then (1) can be rewritten as

$$
\begin{aligned}
H/t_0 = -\sum_{n,s}&[1+(-1)^n(\phi_{n+1}+\phi_n)]\\
&\times(a^\dagger_{n+1,s}a_{n,s}+\text{c.c.})\\
&+\frac{1}{\lambda\pi}\sum_n(\phi_{n+1}+\phi_n)^2+\frac{4}{\lambda\pi}\sum_n(\phi'_n)^2 ,
\end{aligned}
\tag{3}
$$

where $\phi'=d\phi/d\tau$. Equation (3) shows that if energy is measured in units of t_0 and frequency in units of ω_Q, then the properties of the system will only depend on λ.

From Eq. (3) we can see that when $\phi_n=\frac{1}{2}$, the electron states on the chain are split into separated dimers, which will be reached when $\lambda=2/\pi$, so the range of λ is $[0,2/\pi]$. It can also be shown, based on (3), that there is a critical value $\lambda_c=0.2119$; when $\lambda>\lambda_c$, the optical phonon band will no longer overlap with the acoustic phonon band, and it is adequate to take λ_c as the boundary between the weak and strong coupling.

Suppose $\delta\phi_n$ is a small deviation from the equilibrium configuration ϕ_n of the soliton, then the total energy of

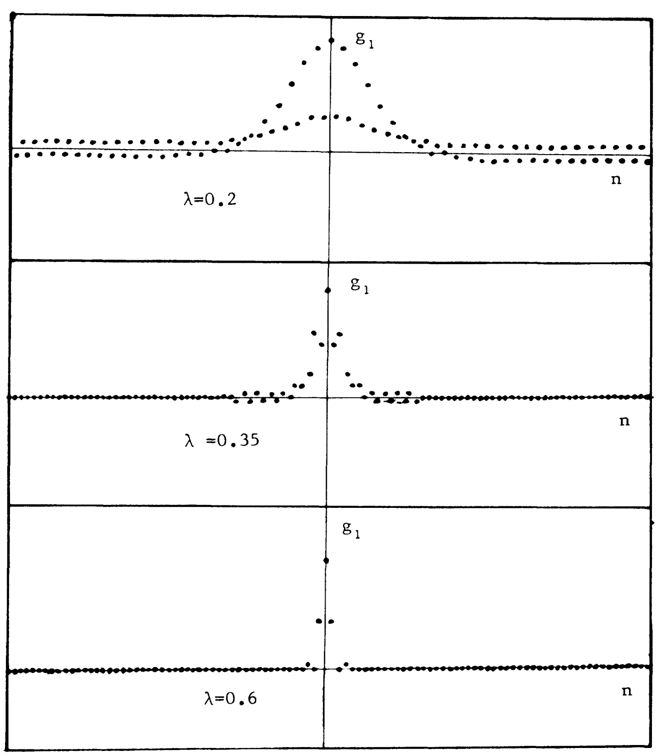

FIG. 1. The evolution of the configuration of g_1 $(0<\lambda<2/\pi)$.

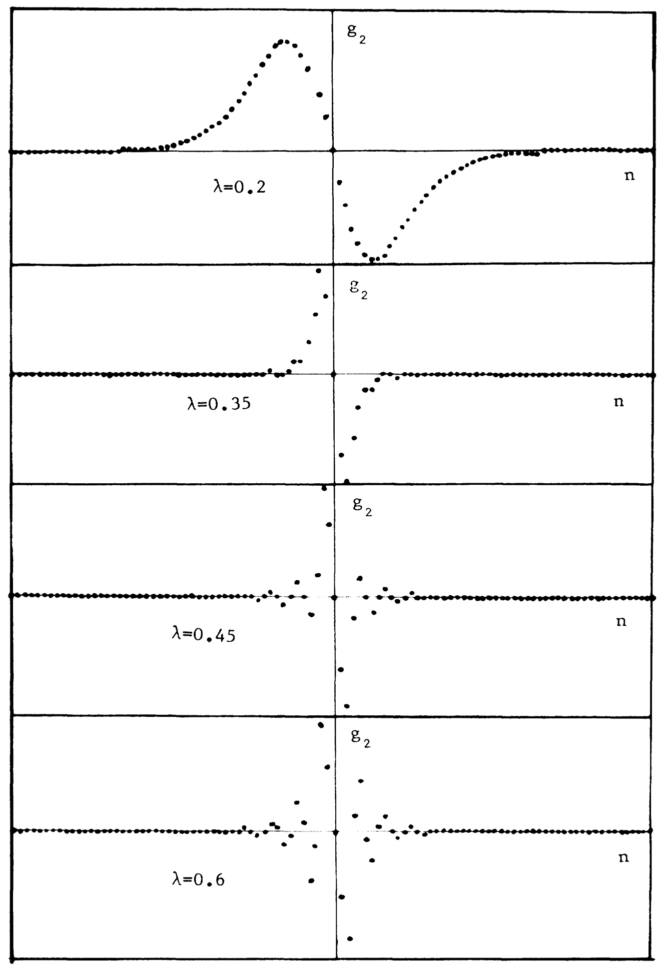

FIG. 2. The evolution of the configuration of g_2 $(0<\lambda<2/\pi)$.

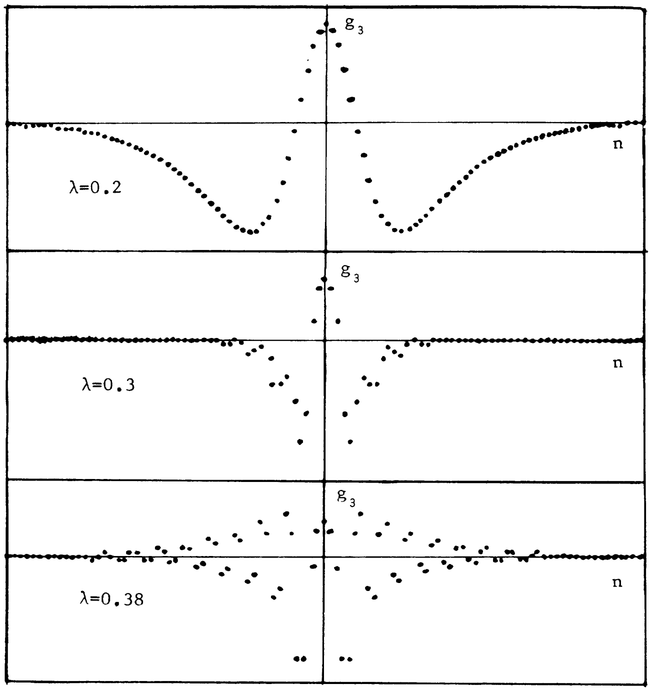

FIG. 3. The evolution of the configuration of g_3 $(0.13<\lambda<0.41)$.

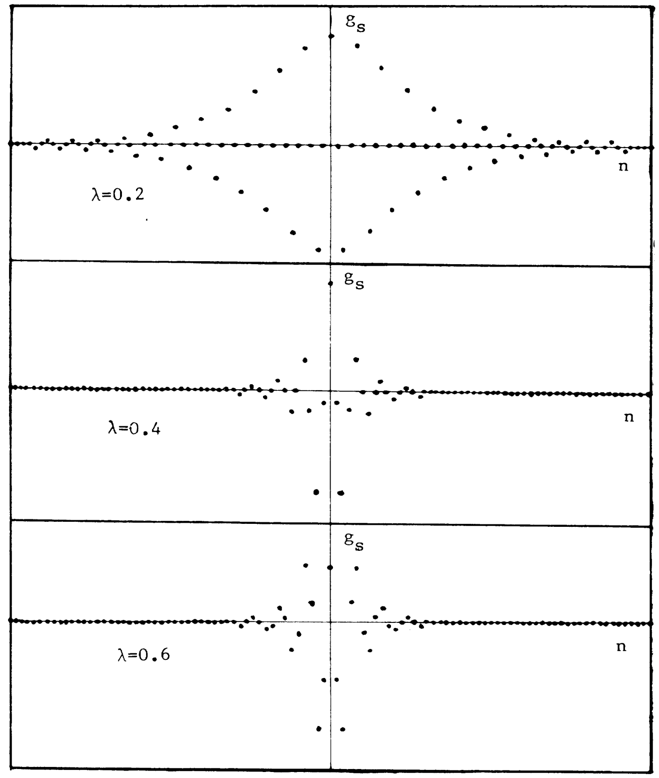

FIG. 5. The evolution of the configuration of g_s $(0<\lambda<2/\pi)$.

the system can be expanded as

$$E(\{\delta\phi_n\})=E_s+\sum_m A_m\delta\phi_m+\tfrac{1}{2}\sum_{m,n}B_{mn}\delta\phi_m\delta\phi_n+4\sum_n(\delta\phi_n')^2+\cdots , \tag{4}$$

where E_s is the energy of the soliton, and

$$A_n=\frac{2}{\lambda\pi}(\phi_{n-1}+2\phi_n+\phi_{n+1})-2(-1)^n\sum_\mu{}' Z_{\mu,n}(Z_{\mu,n+1}-Z_{\mu,n-1}) , \tag{5}$$

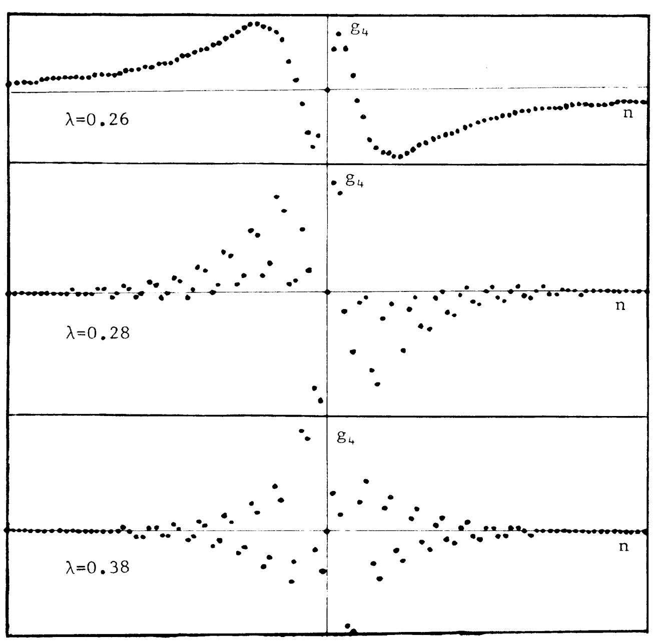

FIG. 4. The evolution of the configuration of g_4 $(0.22<\lambda<0.43)$.

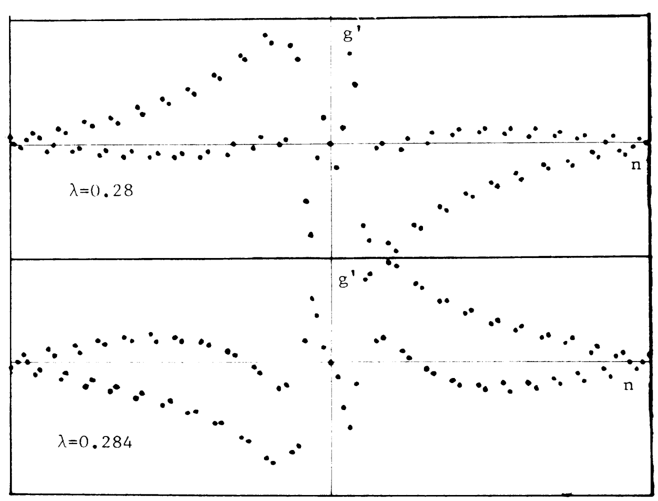

FIG. 6. The evolution of the configuration of g' $(0.276<\lambda<0.284)$.

$$B_{mn}=\frac{2}{\lambda\pi}(\delta_{m,n-1}+2\delta_{m,n}+\delta_{m,n+1})+2(-1)^{m+n}\sum_{\mu}{}'\sum_{\nu}\frac{C^m_{\mu\nu}C^n_{\mu\nu}}{\varepsilon_\mu-\varepsilon_\nu}\;, \tag{6}$$

$$C^m_{\mu\nu}=Z_{\mu,m}(Z_{\nu,m+1}-Z_{\nu,m-1})+Z_{\nu,m}(Z_{\mu,m+1}-Z_{\mu,m-1})\;. \tag{7}$$

Here ε_μ and $Z_{\mu,m}$ are the eigenenergy and eigenfunction of electrons in the static soliton; they are determined by the following self-consistent equations:[10]

$$-[1+(-1)^n(\phi_n+\phi_{n+1})]Z_{\mu,n+1}-[1+(-1)^{n-1}(\phi_{n-1}+\phi_n)]Z_{\mu,n-1}=\varepsilon_\mu Z_{\mu,n}\;, \tag{8}$$

$$\phi_n+\phi_{n+1}=(-1)^n\lambda\pi\left[\sum_{\mu}{}'Z_{\mu,n}Z_{\mu,n+1}-\frac{1}{N}\sum_{n,\mu}{}'Z_{\mu,n}Z_{\mu,n+1}\right]\;. \tag{9}$$

Solving these equations by numerical iterations, we can get the equilibrium configuration ϕ_n of the solitons, and by substituting it into Eq. (6) and diagonalizing B_{mn}, all the vibrational modes will be obtained, and the localized ones can be picked out from these modes.

Our calculations, which were done in a ring consisting of 101 atoms, demonstrate that in a strongly coupled system there can appear six localized modes around the soliton; they are g_1, g_2, g_3, g_4, g_s, and g'. g_1, g_3, and g_s have even parity and they are infrared active; the other three localized modes have odd parity. Among these six localized modes, g_1, g_2, and g_s will always appear for any λ, but g_3, g_4, and g' can only exist for some limited regions of λ; the existing regions and some other properties of the localized modes are shown in Table I. When λ increase, the width of the soliton will shrink, and the configurations of localized modes will change. The evolutions of the configuration for each localized mode are shown in Figs. 1–6. Since the number of the localized modes depends on λ, the whole range $[0,2/\pi]$ of λ will be divided into seven regions, each one with a characteristic disposition of localized modes, which is shown in Table II.

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