Intrinsic localized states and nonlinear excitations of Bloch electrons in electric fields

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Bloch electrons with Coulomb interaction will take localized motion on a discrete lattice in the electric fields. They are always oscillatory in time, with oscillatory frequencies determined by electric fields. Their nonlinear excitations are the spatially localized and time periodic or quasiperiodic, and possess multiple frequencies and comprise multiple soliton components.

This paper addresses the dynamics of Bloch electrons with Coulomb interaction on a discrete lattice in the electric fields. The analysis is based on exact calculations with the inverse scattering method. The results are interesting, and include intrinsic localized states and nonlinear excitations of Bloch electrons. Such a system can be written as an extended Hubbard model,[1] which is relevant to a variety of fields, including exciton states in molecular crystals,[2] oscillations of the sequential tunneling in superlattices,[3] electron excitations in polaronic contexts,[4] and the localized properties of excitations in ferroelectric materials.[5]

The Hamiltonian of the extended Hubbard model is thus

$$H = -V \sum_n \left[\psi_n(t)\psi^*_{n+1}(t) + \psi^*_n(t)\psi_{n+1}(t) \right]$$

$$+ \sum_n nea[\epsilon_d + \epsilon_a \cos(\omega_a t)]|\psi_n(t)|^2$$

$$- U \sum_n \left[|\psi_{n-1}(t)|^2 + |\psi_{n+1}(t)|^2 \right] |\psi_n(t)|^2, \quad (1)$$

with the anticommutation relation $\{\psi_n, \psi_m\} = \{\psi^*_n, \psi^*_m\} = 0$, $\{\psi_n, \psi^*_m\} = \delta_{nm}$, where $|\psi_n(t)|^2$ is proportional to the electron density at site n and time t, V is the nearest-neighbor intersite overlap integral, e is the electron charge, a is the lattice constant, U is the Coulomb interaction between two electrons, ϵ_d and ϵ_a are dc and ac electric fields, and ω_a is the frequency of the ac electric field, respectively. Usually this model is applied to tightly bound orbitals. Then U is quite large, perhaps 10 eV. The bandwidth V is sometimes taken to be smaller. However, some of the most interesting phenomena seem to occur for $U \approx V$. For simplicity, we can choose $U = V = 1$. If we neglect the nonlinearity, the system will reduce to a linear limit; the electron state $\psi_n(t)$ can be expressed as a linear combination of Wannier states.[6] The discreteness of the system gives rise to some interesting features which are not present in the continuum limit.

There has been tremendous progress in the past 30 years in developing analytical methods, such as the inverse scattering method,[7] for finding exact solutions of one-dimensional nonlinear discrete systems.[8] The basic idea of the inverse scattering method is to transform a nonlinear problem into a linear scattering problem. According to the inverse scattering method, the exact single-soliton solution of the extended Hubbard model [Eq. (1)] can be written as

$$\psi_n(t) = \sinh \beta \, \text{sech}[\beta n + 2 \sinh \beta g(t) - \beta n_0]$$

$$\times \exp\left[-inea\left(\epsilon_d t + \frac{\epsilon_a}{\omega_a}\sin(\omega_a t) \right) + i\Omega_c f(t) \right], \quad (2)$$

where $\Omega_c = 2 \cosh \beta$ is the carrier-wave frequency, and β is a constant, while

$$f(t) = A + B + C + \sum_{m=1}^{\infty} J_{2m}\left(\frac{ea\epsilon_a}{\omega_a}\right)\left\{ \frac{\sin[(ea\epsilon_d + 2m\omega_a)t]}{ea\epsilon_d + 2m\omega_a} \right.$$

$$\left. + \frac{\sin\{[ea\epsilon_d - 2m\omega_a]t\}}{ea\epsilon_d - 2m\omega_a} \right\} + \sum_{m=0}^{\infty} J_{2m+1}\left(\frac{ea\epsilon_a}{\omega_a}\right)$$

$$\times \left\{ \frac{\sin[(ea\epsilon_d + (2m+1)\omega_a)t]}{ea\epsilon_d + (2m+1)\omega_a} \right.$$

$$\left. - \frac{\sin[(ea\epsilon_d - (2m+1)\omega_a)t]}{ea\epsilon_d - (2m+1)\omega_a} \right\} \quad (3)$$

and

$$g(t) = J_0\left(\frac{ea\epsilon_a}{\omega_a}\right)\frac{1 - \cos(ea\epsilon_d t)}{ea\epsilon_d}$$

$$+ \sum_{m=1}^{\infty} J_{2m}\left(\frac{ea\epsilon_a}{\omega_a}\right)\left\{ \frac{1 - \cos[(ea\epsilon_d + 2m\omega_a)t]}{ea\epsilon_d + 2m\omega_a} \right.$$

$$\left. + \frac{1 - \cos\{[ea\epsilon_d - 2m\omega_a]t\}}{ea\epsilon_d - 2m\omega_a} \right\} + \sum_{m=0}^{\infty} J_{2m+1}\left(\frac{ea\epsilon_a}{\omega_a}\right)$$

$$\times \left\{ \frac{1 - \cos[(ea\epsilon_d + (2m+1)\omega_a)t]}{ea\epsilon_d + (2m+1)\omega_a} \right.$$

$$\left. - \frac{1 - \cos\{[ea\epsilon_d - (2m+1)\omega_a]t\}}{ea\epsilon_d - (2m+1)\omega_a} \right\}, \quad (4)$$

where

$$A = \begin{cases} J_0\left(\dfrac{ea\epsilon_a}{\omega_a}\right)t & \text{if } \dfrac{ea\epsilon_d}{\omega_a} = 0 \\[2ex] J_0\left(\dfrac{ea\epsilon_a}{\omega_a}\right)\dfrac{\sin(ea\epsilon_d t)}{ea\epsilon_d} & \text{if } \dfrac{ea\epsilon_d}{\omega_a} \neq 0, \end{cases} \quad (5)$$

$$B = \begin{cases} J_{2m}\left(\dfrac{ea\epsilon_a}{\omega_a}\right)t & \text{if } \dfrac{ea\epsilon_d}{\omega_a} = \pm 2m \\ \\ 0 & \text{if } \dfrac{ea\epsilon_d}{\omega_a} \neq \pm 2m, \end{cases} \qquad (6)$$

$$C = \begin{cases} \mp J_{2m+1}\left(\dfrac{ea\epsilon_a}{\omega_a}\right)t & \text{if } \dfrac{ea\epsilon_d}{\omega_a} = \pm(2m+1) \\ \\ 0 & \text{if } \dfrac{ea\epsilon_d}{\omega_a} \neq \pm(2m+1), \end{cases} \qquad (7)$$

and $J_m(ea\epsilon_a/\omega_a)$ $(m=0,\pm 1, \dots)$ are Bessel functions of the first kind, respectively. The corresponding energy, momentum, and norm are

$$E = -4 \sinh \beta, \quad P = 4 \sinh \beta, \quad M = 2\beta. \qquad (8)$$

Equation (2) represents precisely the intrinsic localized state of Bloch electrons on a discrete lattice. The envelope of this soliton is always a hyperbolic secant, and it is the same as that of the continuum case, but the motion of its center is different from the continuum case.[9] When the external electric fields are zero, we find that, in contrast to the diffusing motion of Bloch electrons for the potential-free case in the linear limit,[6] Bloch electrons will take localized motion under the action of nonlinear Coulomb interaction U. These are the intrinsic localized states.

We can readily show that this single-soliton solution has a continuous translational symmetry on account of the arbitrariness of n_0. If we omitted the nonlinear strength U, the equation of motion of Bloch electrons is invariant under the following transformations: if $\psi_n \rightarrow (-1)^n \psi_n$, $t \rightarrow -t$ for the potential-free case or the electric field as any odd function of time, there exist "staggered" localized states. In this case, the system possesses the following reflectional symmetry: if an unstaggered state $\psi_n e^{i\omega_a t}$ is a solution of the system, then the staggered state $(-1)^n \psi_n e^{i\omega_a t}$ is also a solution of the system. Under reflectional transformation, the single-soliton solution [Eq. (2)] transforms to a set of solutions identical to the original set in Eq. (2), but with a different parametrization. It follows that this single-soliton solution possesses the exact self-dual reflectional symmetry.

As a generalization of the well-known linear case,[6] the single-soliton solution [Eq. (2)] is always oscillatory in time and bounded, i.e., the oscillatory of Bloch electrons with Coulomb interaction in dc-ac electric fields is periodic, while the oscillatory frequencies are determined by the coupling of the magnitude ϵ_d of the dc electric field and the frequency ω_a of the ac electric field.[10]

For the case of a dc electric field, it can be readily seen that the single-soliton solution [Eq. (2)] oscillates in time. This means that Bloch electrons with Coulomb interaction in a dc electric field will move as periodic oscillations; the so-called "Bloch oscillations" with Bloch frequency $\omega_B = ea\epsilon_d$. This oscillation frequency is determined by the strength of the dc electric field. This is exactly the well-known result obtained first by Zener.[11] As a generalization of the linear case, this soliton solution is a bounded and periodic solution, and it is different from that for a continuum

case. It is concluded that in the limit of a dc electric field, the system exhibits a periodic evolution which is a nonlinear counterpart of Bloch oscillations.[12] This nonlinear Bloch oscillation has been found in experiments of waveguide arrays.[13]

If an ac electric field alone exists, we can easily find that the single-soliton solution [Eq. (2)] oscillates with the period $T = 2\pi/\omega_a$ in time and remains bounded, and its oscillatory period is the same with that of an ac electric field. This means that Bloch electrons are effectively localized by the action of an ac electric field. If Bloch electrons are initially localized in space, they can be dynamically trapped by an ac electric field.

As a measure of localization, we can introduce the mean width W of a pulse,

$$W = \left(\frac{\displaystyle\sum_{n=-\infty}^{\infty} n^2 |\psi_n(t)|^2}{\displaystyle\sum_{n=-\infty}^{\infty} |\psi_n(t)|^2} \right)^{1/2}, \qquad (9)$$

where the pulse center is assumed to be at a site $n=0$. Thus for a complete localization of the energy at the center site, W becomes zero. The oscillations of W are $\pi/2$ out of plane, due to norm conservation. We can find the time evolution of the mean width of a pulse exhibiting a localization of Bloch electrons with Coulomb interaction in dc-ac electric fields. The mean width W of a pulse is oscillatory, and a monotonical decrease does not exist as time changes. This is different from the initial phase of a blowup in the continuum system. We note again that the mean width of the pulse never reaches zero.

Summing up the previous discussions, we should emphasize the differences between the ac and dc-ac cases for intrinsic localized states and oscillations. In the ac case the oscillation period is the same as that of an ac electric field. However, in the dc-ac case the situation is quite different. Oscillation frequencies are determined by a coupling of the magnitude ϵ_d of a dc electric field and the frequency ω_a of an ac electric field. They have nothing to do with the magnitude ϵ_a of an ac electric field. We believe such a character may be related to Wannier-Stark ladders,[14] because of the effect of a dc field.

The two-soliton solutions $\psi_n(t)$ can be written as

$$\psi_n(t) = \frac{\sinh(2\beta)[C_1 + C_2 \exp(i\Omega_b f(t))]}{C_3 + (\Omega_c^2 - 1)\cos[\Omega_b f(t)]} \exp\left[-inea\left(\epsilon_d t \right.\right.$$
$$\left.\left. + \frac{\epsilon_a}{\omega_a}\sin(\omega_a t)\right) + i\Omega_c f(t)\right], \qquad (10)$$

where $\Omega_b = 4\sinh(2\beta)\sinh\beta$ represents the shape-mode frequency, and C_i $(i=1,2,3)$ are functions of $g(t)$, respectively. The corresponding energy, momentum, and norm are

$$E = -\frac{4\sinh^2(2\beta)}{\sinh\beta}, \quad P = \frac{4\sinh^2(2\beta)}{\sinh\beta}, \quad M = 8\beta. \qquad (11)$$

Equation (10) is a spatially localized and time periodic breather solution. This breather is a nonlinear composite excitation comprising two-soliton components. It can be viewed as a discrete generalization of two-soliton continuum solutions in the presence of dc-ac electric fields. In the sense of an inverse scattering transformation, Eq. (10) can also be viewed as a breather comprising two single-soliton components with their poles at $e^{-\beta/2}$ and $e^{-3\beta/2}$, respectively. However, this breather will be acted upon by the general discrete effect, then break up into two spatially separating coherent structures undergoing bounded individual motions; in addition, it has a continuous translational symmetry on account of the arbitrariness of n_0.

For the case of external electric fields at zero, Eq. (10) is a discrete breathing soliton solution which has a carrier wave frequency Ω_c and a fundamental shape-mode frequency Ω_b. Its center translates into a parabolic trajectory in time. Similar to that of the continuum case, this breather can be viewed as a particle with an internal degree of freedom, and it will accelerate down a ramp just as a Newtonian particle will do. In general, the two frequencies Ω_c and Ω_b are incommensu-

rate; the breather [Eq. (10)] is not periodic in time. Only when these two frequencies are commensurate with each other can the breather [Eq. (10)] become a periodic solution. This is the resonance issue of a Bloch electron with Coulomb interaction.

If only a dc electric field exists, we can conclude that the evolution of the discrete breather [Eq. (10)] is still periodic with a period $2\pi/ea\epsilon_d$. However, this breather no longer evolves as a single coherent entity for the discreteness effect. It breaks up into two spatially separating lumps with coherent structures: one with a stable envelope and the other with a time dependent envelope. Only under the conditions $\beta^2 \ll 1$ and $t \ll 1/ea\epsilon_d$ can we separate this discrete breather to that of the continuum case. When the parameter β increases, these two lumps separate more prominently.

For the case of an ac electric field, we can easily find that this breather also breaks up two lumps for a general discrete effect. In general, the motion of Bloch electrons with Coulomb interaction in an ac electric field is no longer periodic.

The final exact results for the wave function $\psi_n(t)$ as a three-soliton solution can be written as

$$\psi_n(t) = \sinh(3\beta) \frac{C_1 + C_2 \exp[i\Omega_{b1}f(t)] + C_3 \exp[i\Omega_{b2}f(t)] + C_4 \exp[i(\Omega_{b2}-\Omega_{b1})f(t)] + C_5 \exp[-i(\Omega_{b2}-\Omega_{b1})f(t)]}{C_6 + C_7 \cos[\Omega_{b1}f(t)] + C_8 \cos[\Omega_{b2}f(t)] + C_9 \cos[(\Omega_{b2}-\Omega_{b1})f(t)]}$$

$$\times \exp\left[-inea\left(\epsilon_d t + \frac{\epsilon_a}{\omega_a}\sin(\omega_a t)\right) + i\Omega_c f(t)\right], \tag{12}$$

where $\Omega_{b1} = 2[\cosh(3\beta) - \cosh\beta]$ and $\Omega_{b2} = 2[\cosh(5\beta) - \cosh\beta]$ represent two shape-mode frequencies, and C_i ($i = 1, \ldots, 9$) are functions of $g(t)$, respectively. The corresponding energy, momentum, and norm are

$$E = -\frac{4\sinh^2(3\beta)}{\sinh\beta}, \quad P = \frac{4\sinh^2(3\beta)}{\sinh\beta}, \quad M = 18\beta. \tag{13}$$

Equation (12) can be viewed as a discrete breather which evolves with three fundamental frequencies; a carrier wave frequency Ω_c and two fundamental shape-mode frequencies Ω_{b1} and Ω_{b2}. A discrete breather possessing multiple frequencies is conceptually important in studies of nonlinear lattice systems. In the sense of an inverse scattering transformation, Eq. (12) can also be viewed as a breather comprising three single-soliton components with their poles at $e^{-\beta}$, $e^{-3\beta}$, and $e^{-5\beta}$, respectively. Generally, these two shape-mode frequencies Ω_{b1} and Ω_{b2} are incommensurate; therefore, the envelope of the breather does not have a temporally periodic evolution, and this nonlinear excitation cannot be decomposed into three periodic components. This is an example of a spatially localized, temporally quasiperiodic, nonlinear breathing structure. The incommensurability of the breather frequencies is a discrete lattice effect. When three fundamental frequencies satisfying some special relations, for example, $\Omega_c:\Omega_{b1}:\Omega_{b2} = 1:8:24$ in the limit of $\beta \to 0$,

these frequencies become commensurate in the continuum limit; the evolution of the continuum breather is always periodic in time. This is the resonant situation of Bloch electron with Coulomb interaction.

Equation (12) possesses a continuous translational symmetry, that is, n_0 is an arbitrary real number, and the corresponding energy, momentum, and norm [Eq. (13)] are independent of n_0. The energy, momentum, and norm are simple arithmetic sums of the three single solitons with their poles at $e^{-\beta}$, $e^{-3\beta}$, and $e^{-5\beta}$. We find that Eq. (12) is a special kind of bound state with null binding energy and norm. Therefore, it is marginally stable and may decay into three-soliton components under perturbation. Moreover, as a more significant property of the solution, Eq. (12) is stable after a collision with a soliton.

When the external electric field is at zero, Eq. (12) is a discrete breathing soliton solution which has a carrier wave frequency Ω_c and two fundamental shape-mode frequencies Ω_{b1} and Ω_{b2}. Its center translates in a parabolic trajectory in time. Similar to the continuum case, this breather can be viewed as a particle with an internal degree of freedom, and it will accelerate down a ramp just as a Newtonian particle will do. In general, the two shape-mode frequencies Ω_c and Ω_b are incommensurate; this breather is not periodic in time. When these two shape-mode frequencies become commensurate, this breather is always a periodic solution. This is the

resonance issue of a Bloch electron under the action of the nonlinear effect.

If only a dc electric field exists, this breather no longer evolves as a single coherent entity for the discreteness effect. It breaks up into three spatially separating lumps with coherent structures, one with a stable envelope and the other with a time-dependent envelope. When the parameter β increases, these two lumps separate more prominently. Only under the conditions $\beta^2 \ll 1$ and $t \ll 1/ea\epsilon_d$ can we recover the continuum solution from this discrete breather under the action of a dc electric field. Of course, the evolution of the discrete breather is still periodic with a period $2\pi/ea\epsilon_d$.

When only an ac electric field exists, we can easily find that this breather also breaks up three lumps for a general discrete effect. In general, the motion of Bloch electrons with Coulomb interaction in an ac electric field is no longer periodic.

The N soliton solutions $\psi_n(t)$ can be written as

$$\psi_n(t) = \frac{\sinh(N\beta) \sum_{l=1}^{2N-1} C_l \exp[i(\Omega_{b(l-1)} - \Omega_{b(l-2)})f(t)]}{\sum_{m=1}^{2N-2} C_m \cos[(\Omega_{b(m-1)} - \Omega_{b(m-2)})f(t)]}$$

$$\times \exp\left[-inea\left(\epsilon_d t + \frac{\epsilon_a}{\omega_a}\sin(\omega_a t)\right) + i\Omega_c f(t)\right],$$

(14)

where $\Omega_{bl} = 2\{\cosh[(2l+1)\beta] - \cosh\beta\}$ represents the lth shape-mode frequency. The corresponding energy, momentum, and norm are

$$E = -\frac{4\sinh^2(N\beta)}{\sinh\beta}, \quad P = \frac{4\sinh^2(N\beta)}{\sinh\beta}, \quad M = 2N^2\beta.$$

(15)

Equation (14) is a discrete breathing soliton solution which has a carrier wave frequency Ω_c and $N-1$ fundamental shape-mode frequencies Ω_{bl} ($l = 1, 2, \ldots, N-1$). In general, any two frequencies $\Omega_{(l-1)}$ and Ω_l are incommensurate, this breather is not periodic in time. When any two frequencies become commensurate, this breather is always a periodic solution. This is the resonance issue of Bloch electrons with Coulomb interaction.

Equation (14) is a nonlinear composite excitation comprising N soliton components. It can be viewed as a discrete generalization of N soliton continuum solutions in the presence of dc-ac electric fields. In the sense of an inverse scattering transformation, Eq. (14) can also be viewed as a breather comprising N soliton components with their poles at $e^{-\beta/2}$, $e^{-3\beta/2}$, $\ldots$, $e^{-[(l-1)\beta/2]}$, $\ldots$, $[l = 1, 2, \ldots, (N-1)]$, respectively. However, this breather will be acted upon by the general discrete effect, and will then break up into N spatially separating coherent structures undergoing bounded individual motions; in addition it has a continuous translational symmetry on account of the arbitrariness of n_0.

For a clear and better understanding on the dynamics of Bloch electrons, the properties associated with the effects of the ac and dc electric fields could be summarized as the follows: Bloch electron: dc fields, ac fields, dc-ac fields. Motion of electron: localized-localized-localized. Staggered states: no $\psi_n \to (-1)^n \psi_n$ and $\psi_n \to (-1)^n \psi_n$. Oscillatory frequency: $\omega_B = ea\epsilon_d$ and $\omega_a = ea\epsilon_d + 2m\omega_a$.

In conclusion, the dynamics of Bloch electrons with Coulomb interaction on a discrete lattice in dc-ac electric fields has many interesting features, which were beyond the reach of the linear limit and the continuum limit. In the sense of an inverse scattering transformation, these breathers are bona fide soliton solutions. They are actually discrete generalizations of the continuum multiple-soliton solutions. These breathers, with incommensurate internal breathing frequencies, exist only in the discrete lattice. They approach time periodic solutions in the continuum limit. They are important for an understanding of spatially localized nonlinear excitations in certain classical and quantum systems.

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