Effects of off-diagonal nonlinearity on the time evolution of an initially localized mode

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A modified one-dimensional nonlinear Schrödinger equation which includes off-diagonal nonlinearity is proposed to describe the behavior of electrons via electron-phonon couplings in the Su-Schrieffer-Heeger Hamiltonian. We find an interesting self-trapping phenomenon of electrons which takes place when the magnitude of the nonlinearity parameter is close to the value of the hopping integral. For a periodic lattice, the ballistic propagation of a wave packet is found in this modified one-dimensional nonlinear Schrödinger equation, and the propagation rate increases with the increase of nonlinearity parameter except in the self-trapping interval. When diagonal disorder is introduced, the electronic states are localized, and no delocalization effect of the off-diagonal nonlinearity is found. These results are quite different from that in the diagonal nonlinear lattice, where delocalization is found. [S1063-651X(97)10209-4]

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I. INTRODUCTION

The study of the interplay of disorder and nonlinearity is of great importance in a variety of fields in condensed-matter physics. Both are regarded as origins of the localization, and have received much attention since the last decade [1,2]. The theory of Anderson localization predicts that the wave function of an electron moving in a one-dimensional lattice with on-site energy disorder is localized even for an infinitesimal amount of disorder [3–7]. Thus in such systems the mobility of electrons is inhibited. On the other hand, nonlinearity arises, for example, from the interaction between electrons and lattice vibrations [8]. This leads to the possibility of the occurrence of a mobility edge [9]. Furthermore, the interaction between electrons and lattice vibrations can lead to an effective correlation between the site energy and the nearest-neighbor overlap integral, thus resulting in possible delocalization [10]. The most widely used equation describing the motion of an electron in a one-dimensional lattice with electron-phonon interaction is the discrete nonlinear Schrödinger equation (DNLSE) [11–14]

$$i\dot{c}_n=\epsilon_n c_n+V(c_{n+1}+c_{n-1})-\chi_n|c_n|^2c_n, \qquad (1)$$

where c_n is the wave amplitude at site n, V is the hopping integral between nearest-neighbor sites, ϵ_n is the on-site energy, and χ_n is a nonlinearity parameter which is proportional to the local electron-phonon coupling under an adiabatic approximation [15]. From the above DNLSE we can see that when $\chi_n=0$, and the on-site energy is randomly distributed, it reduces to the Anderson model, where all the eigenstates of electrons are localized [3,4]. In dynamics, an initially localized mode will remain localized in a finite region, and the time-averaged probability to find the particle at the initial site will be significantly larger than 0. However, if nonlinearity and the randomness in the site energies coexist, the dynamical localization will be destroyed by nonlinearity. Shepelansky found that when the nonlinearity parameter is greater than a critical value $\chi_{n_{\rm cr}}$, the motion of a wave packet will be subdiffusive for large time [16]. Recently, Molina and Tsironis introduced a nonlinear random binary alloy (NRBA) model [17], where two species of sites with different nonlinearity parameters are randomly distributed, and the disorder resides completely in the nonlinear term. They studied the dynamical localization of the NRBA, and found the absence of electronic localization except for a very large nonlinearity parameter. The presence of disorder is completely overcome by the nonlinear term, leading to ballistic propagation of the untrapped fraction of the electrons.

Another important property of the DNLSE is the self-trapping phenomenon [11,18–20], i.e., the clustering of the electron amplitude on a single site. When the nonlinearity parameter is greater than the critical value $4V$, self-trapping occurs. Thus the probability of finding the particle at the initial site is always nonzero.

The electron-phonon interaction included in the DNLSE describes the lattice vibrations coupled to the diagonal electronic matrix element of the electron Hamiltonian, we call this diagonal nonlinearity. In fact, the lattice vibration can also be coupled to the off-diagonal electronic matrix elements [21]. It is then interesting to investigate the combined effects of disorder and off-diagonal nonlinearity on the localization and transport properties of a low-dimensional condensed-matter system.

In this paper we investigate the self-trapping and the dynamical localization property of a modified nonlinear Schrödinger equation (MNLSE) which is proposed to describe the off-diagonal nonlinearity caused by the electron-phonon coupling in a Su-Schrieffer-Heeger (SSH) Hamiltonian. In Sec. II of this paper we describe the origin of the MNLSE from the SSH Hamiltonian. In Sec. III we study the dynamical properties of the MNLSE in a periodic lattice, and in Sec. IV we investigate the combined effects of off-diagonal nonlinearity and on-site energy disorder on the localization of electrons. In Sec. V we give a brief summary.

II. MODEL

We consider an electron moving in polyacetylene or other polymers. When we take into account the interaction be-

tween the π electrons and the lattice vibrations, we can use the SSH Hamiltonian [21]

$$H=\tfrac{1}{2}M\sum_n |\dot{u}_n|^2+\tfrac{1}{2}K\sum_n (u_n-u_{n+1})^2$$

$$-\sum_n (t_0+\alpha(u_n-u_{n+1}))(c_n^\dagger c_{n+1}+c_{n+1}^\dagger c_n), \quad (2)$$

where u_n is the displacement of lattice, t_0 is the intrinsic hopping integral, α is the electron-phonon coupling constant, and c_n is the electron probability amplitude at site n.

From a variational calculation with the adiabatic approximation, it is found that the displacement of each bond is proportional to local electron density at its ends. Substituting this into the expression of the SSH Hamiltonian yields an equation of motion of electrons, the MNLSE:

$$i\dot{c}_n=\epsilon_n c_n+V(c_{n+1}+c_{n-1})+v_n(|c_n|^2+|c_{n+1}|^2)c_{n+1}$$
$$+v_n(|c_n|^2+|c_{n-1}|^2)c_{n-1}, \quad (3)$$

where v_n is a parameter describing the electron-phonon coupling, and ϵ_n is the on-site energy which is added to the equation.

The dynamical properties of the MNLSE can be investigated by considering the time evolution of a wave packet which is initially localized at site n_0:

$$c_n(0)=\delta_{n,n_0}. \quad (4)$$

The propagation of the wave packet can be characterized by several quantities. One of them is the time-dependent probability to find the particle at the initial site,

$$W_0(t)=|c_{n_0}(t)|^2, \quad (5)$$

and the others are the mean square displacement (MSD) and the participation number, which are defined as

$$(\Delta n(t))^2=\sum_n (n-n_0)^2|c_n(t)|^2, \quad (6)$$

$$P(t)=\left[\sum_n |c_n(t)|^4\right]^{-1}, \quad (7)$$

respectively.

The root-mean-square displacement usually follows a power law

$$\Delta n(t)\sim t^\gamma. \quad (8)$$

When $\gamma=0$ the wave packet is localized, when $0<\gamma<\frac{1}{2}$ it is subdiffusive, $\gamma=\frac{1}{2}$ corresponds to a diffusive behavior, $\frac{1}{2}<\gamma<1$ corresponds to a superdiffusive behavior, $\gamma=1$ means that the motion is ballistic, and $\gamma>1$ means it is superballistic. The participation number $P(t)$ gives a rough estimation of the number of sites where the wave packet has a significant amplitude. When $P=1$, the wave packet is completely localized, and when $P=N$, the wave packet is uniformly distributed over the whole lattice corresponding to a completely extended behavior.

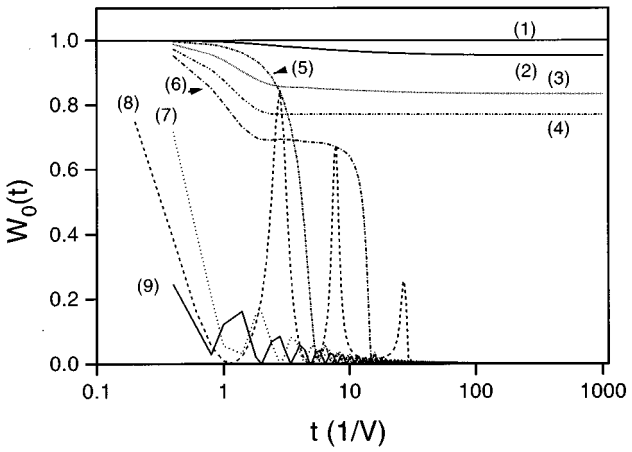

FIG. 1. The time evolution of the return-to-initial site probability $W_0(t)$ in a periodic lattice for different nonlinearity parameters. The nonlinearity parameters for curves (1)–(9) are $-1.0V$, $-1.05V$, $-1.2V$, $-1.3V$, $-0.9V$, $-1.4V$, 0, $-3.0V$, and $1.05V$, respectively. Curves (1)–(4) represent self-trapping states, other curves decay rapidly.

In order to obtain the above quantities, the fourth-order Runge-Kutta method is employed to numerically integrating the MNLSE. To avoid the end effects, the system should be large enough to ensure that the wave amplitude near the boundaries satisfies $|\psi_n|^2<10^{-30}$ during the integration. The integration step is determined in the following way: we stop decreasing the step until the integration results do not change (normally for 5–6 significant digits) with the variation of the step.

III. DYNAMICAL PROPERTIES OF THE MNLSE IN A PERIODIC LATTICE

In this section we will concentrate on the dynamical properties of the MNLSE in a periodic lattice. The lattice we study consists of 5000 sites. Without loss of generality we set all the on-site energies equal to zero in this section, and v_n takes an identical value for all bonds. Since the transformation $(V,v_n)\rightarrow(-V,-v_n)$ only turns the MNLSE into an equation for the complex conjugate variable $c_n^*(t)$, and as a result the site probability $\rho_n=c_nc_n^*=|c_n|^2$ remains invariant, it is then sufficient to take $V>0$ and consider two possible signs of v_n. For the sake of convenience, we set $V=1$. The particle is initially localized on the central site $n_0=2500$.

We calculate the time evolution of the probability to find the electron at the initial site, the mean-square displacement, and the participation number of the system for different nonlinearity parameters. The results are shown in the following figures.

In Fig. 1 we show how the probability of finding the particle at the initial site $W_0(t)$ varies with time for different nonlinearity parameters. From Fig. 1 we can see that $W_0(t)$ always approaches zero when $v_n>0$. But for large nonlinearity parameters, $W_0(t)$ oscillates for some time before decaying to zero. No self-trapping occurs when the nonlinearity parameter is positive.

When v_n is negative, $W_0(t)$ keeps a relatively large value at the initial site for some time, and then decays rapidly to

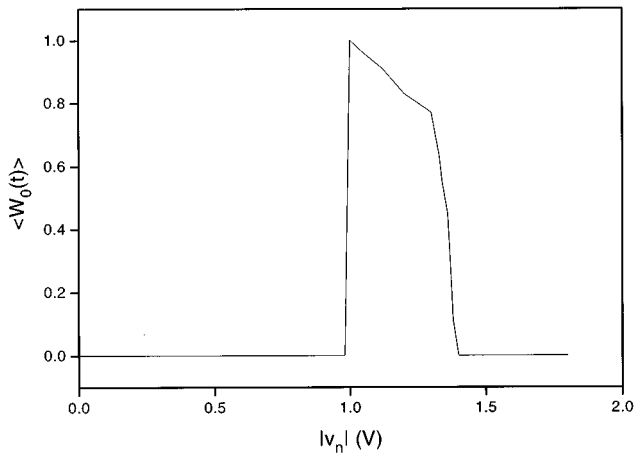

FIG. 2. The dependence of the time-averaged initial-site probability $\langle W_0(t)\rangle$ on nonlinearity parameters. When $|v_n|$ is less than V, $\langle W_0(t)\rangle$ is zero. When $|v_n|$ is greater than $1.4V$, it is again zero. We can see rapid changes of $\langle W_0(t)\rangle$ at $|v_n|=V$ and $|v_n|=1.4V$.

zero. When the magnitude of the nonlinearity parameter increases toward V, the length of this transient time increases until it becomes infinite when $|v_n|=V$, and the probability of finding the particle at the initial site rapidly approaches a constant which is significantly larger than 0. When $|v_n|>V$ and $|v_n|$ is less than an upper critical value v_c, this phenomenon still exists. However, when $|v_n|$ is larger than v_c, the initial-site probability decays to zero after a transient time. Again, this transient time decreases when $|v_n|$ increases from v_c.

In order to determine the value of v_c, we calculate the time-averaged probability of finding the particle at the initial site for different nonlinearity parameters,

$$\langle W_0(t)\rangle = \lim_{T\to\infty} \frac{1}{T}\int_0^T |c_{n_0}(t)|^2 dt, \tag{9}$$

and show the dependence of $\langle W_0(t)\rangle$ on v_n in Fig. 2. In the figure we can see that there is a rapid growth of $\langle W_0\rangle$ at $|v_n|=V$, and it drops to zero at $|v_n|=1.4V$. Thus $v_c=1.4V$, which is determined from the condition $\langle W_0(t)\rangle=0$, and v_c only slightly depends on the number of sites in our numerical studies. Only when v_n is negative and the magnitude of it lies in the interval $(V,1.4V)$ does the self-trapping occur. When $v_n=-V$, $W_0(t)$ is exactly equal to 1.0 at any time. This means that the particle is completely trapped on the initial site when $v_n=-V$. We can see from the MNLSE that it is possible for the right-hand side of the equation to be zero when $v_n<0$. When $v_n=-V$, the right-hand site of the MNLSE is zero at the initial time, and does not change forever, resulting in the constant $\langle W_0(t)\rangle=1.0$. The result for this off-diagonal nonlinearity is quite different from the results of previous work on diagonal nonlinearity [11,18–20]. For diagonal nonlinearity, self-trapping becomes more and more eminent with the increase of the nonlinearity parameter.

In Fig. 3 we demonstrate the root-mean-square displacement of the wave packet as a function of time for different nonlinearity parameters. Numerical studies show that, for large time, the wave packet propagates ballistically despite the sign and magnitude of v_n. In this nonlinear lattice with off-diagonal nonlinearity, the velocity of the wave packet is greater than $\sqrt{2}$, the propagation rate for the linear periodic lattice. Also this rate increases with the increase of nonlinearity parameter when it lies outside the self-trapping interval. If we take a closer look at the detail of the time evolution of the wave packet (see the inset of Fig. 3), we can see that, in this nonlinear lattice, the wave packet propagates ballistically at a rate less than that in linear lattice when t is less then a value t_1. After this time instant, the curve bends over, showing a slope larger than $\sqrt{2}$, and then $\Delta n(t)$ grows linearly with time at this rate. Conversely, in the diagonal nonlinearity case, the rate is smaller than $\sqrt{2}$, and decreases with the increase of the nonlinearity parameter [22]. In the MNLSE, when self-trapping occurs, most of the wave packet is trapped, but the untrapped portion escapes ballistically with a relatively slower velocity. However, when $v_n=-V$, the velocity is zero since the wave packet is wholly trapped in the initial site. The fact that the motion is ballistic even when self-trapping occurs can be understood as follows:

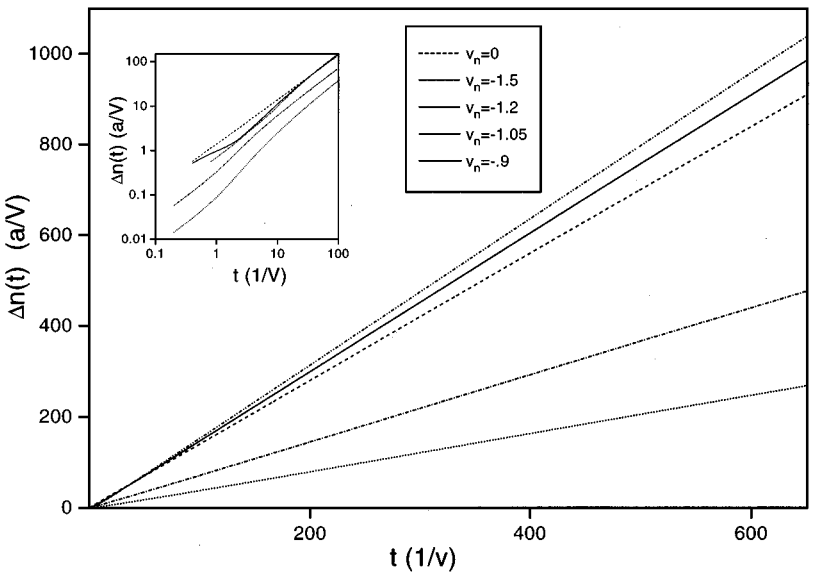

FIG. 3. The root-mean-square displacement of the wave packet as a function of time for different nonlinearity parameters. The unit of $\Delta n(t)$ is a/V, where a is the lattice spacing. The inset is the detail at the beginning. We can see that when no self-trapping occurs, the propagation rate of the wave packet is greater than that in linear lattice, and the propagation is ballistic even when self-trapping occurs.

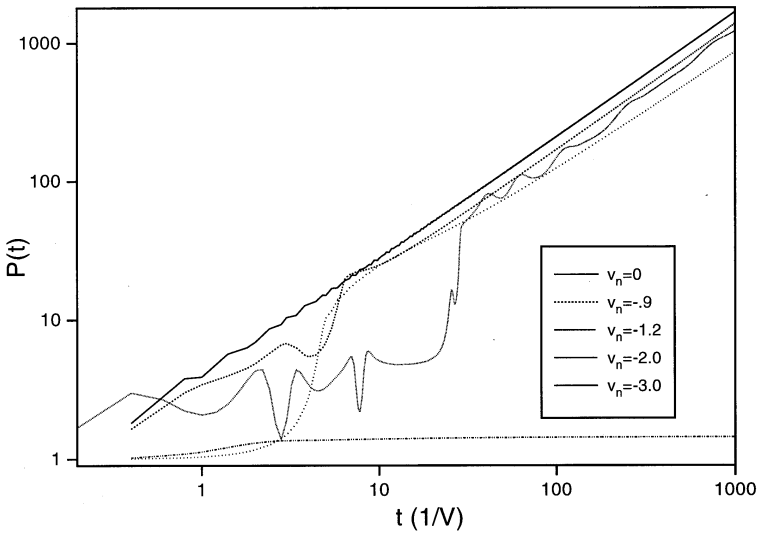

FIG. 4. The participation number $P(t)$ as a function of time for different nonlinearity parameters.

when self-trapping occurs, there is some portion of the probability amplitude escaping from the initial site before the self-trapped state is formed. This escaping portion is relatively small, especially on sites other than the initial site. Thus, because of the smallness of the nonlinear terms in the MNLSE, the motion of this escaping portion is weakly affected by the nonlinearity. The propagation rate of the wave packet is smaller when self-trapping occurs because of the decrease of the escaping portion.

Figure 4 shows how the participation number $P(t)$ of the system varies with time for different nonlinearity parameters. We can see that in the linear case it grows linearly with time, indicating a uniform spreading of the wave packet over the chain. In the nonlinear case we find that when the nonlinearity parameter lies outside the self-trapping interval, the participation number oscillates quickly at first, after a long time the oscillation becomes smaller, and then $P(t)$ grows linearly with time. When the nonlinearity parameter increases,

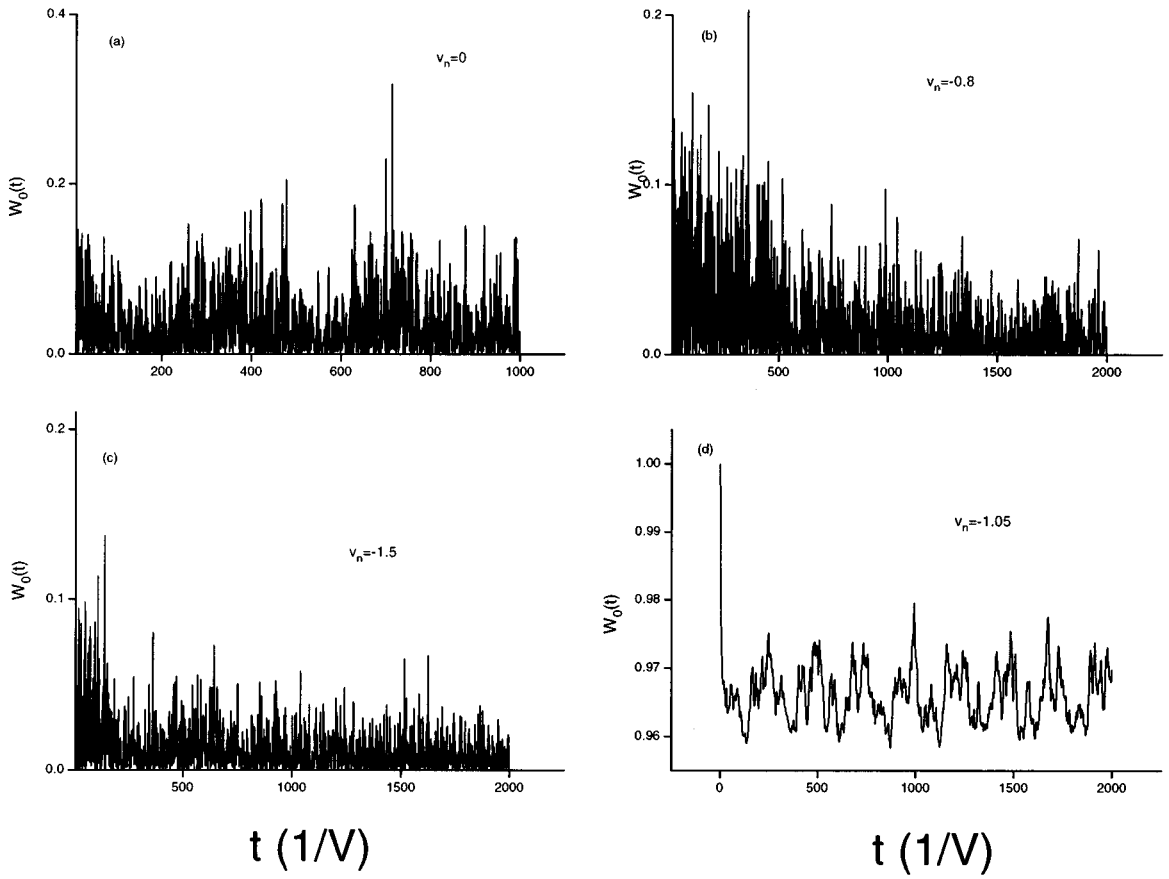

FIG. 5. $W_0(t)$ as a function of time for different nonlinearity parameters with on-site energy disorder. In (a)–(d), the probability is always nonzero, indicating a localized mode. In (d), the probability is very close to 1.0.

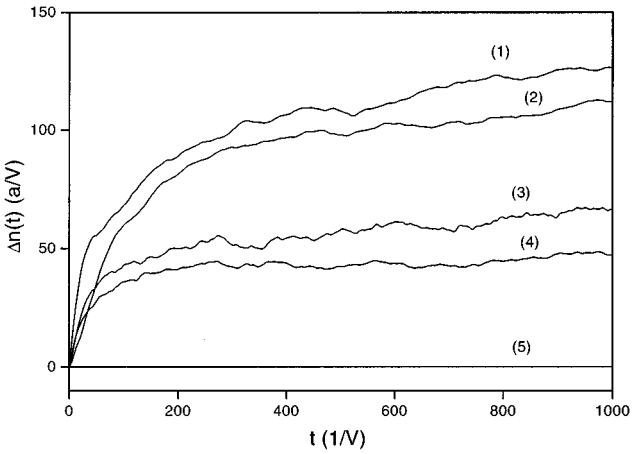

FIG. 6. Root-mean-square displacement vs time in a disordered lattice for different nonlinearity parameters. The unit of $\Delta n(t)$ is a/V, where a is the lattice spacing. The nonlinearity parameters for curves (1)–(5) are $-10.0V$, $-4.0V$, $-0.8V$, 0, and $-1.0V$, respectively. It grows rapidly at first and then saturates.

$P(t)$ oscillates even more dramatically. When v_n is outside but close to the self-trapping interval, $P(t)$ is quite small at first, then abruptly ''climbs'' to a much larger value, and then begins to grow linearly. When nonlinearity parameter is within the self-trapping region, the participation number is very small (close to 1.0), indicating the existence of a trapped mode.

IV. DYNAMICAL PROPERTIES OF THE MNLSE IN A DISORDERED LATTICE

In order to investigate the combined effect of off-diagonal nonlinearity and diagonal disorder on the localization, we set the on-site energy in the MNLSE randomly distributed within the interval $(-0.5V,0.5V)$, and the nonlinearity parameter is taken to be identical for every bond. The intrinsic hopping integral V is set to 1. The number of lattice sites is 5000. The wave packet is initially localized on the 2500th site, and we choose open boundary conditions.

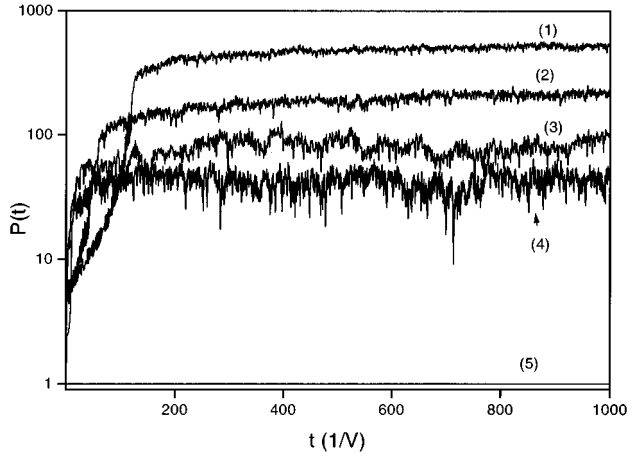

FIG. 7. Participation number vs time in disordered lattice for different nonlinearity parameters. The nonlinearity parameters for curves (1)–(5) are $-20.0V$, $-10.0V$, $-1.5V$, 0, and $-1.0V$, respectively.

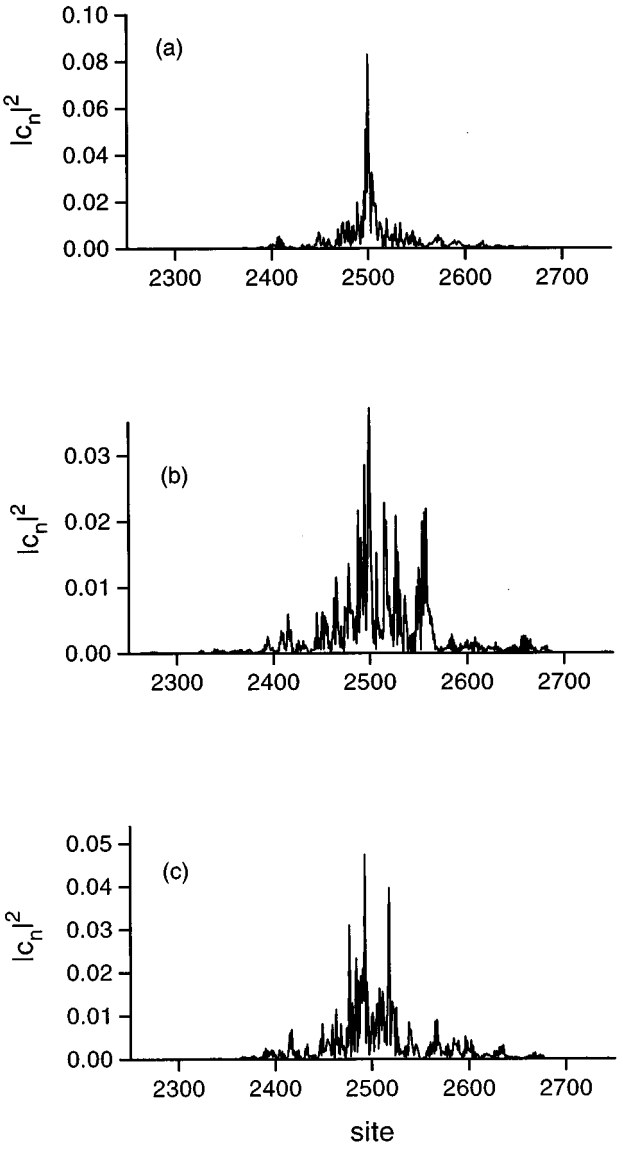

FIG. 8. The spatial distribution of a wave packet for fixed nonlinearity parameters $v_n=-0.9V$ at different time instants for a disordered lattice. (a) $Vt=100$. (b) $Vt=500$. (c) $Vt=1000$. The spatial distribution is within a finite region, and it changes little with time.

The return-to-initial-site probability is shown in Fig. 5. In this figure we can see that there is always a finite probability to find the particle at the initial site no matter the magnitude of the nonlinearity parameter. The results change little when the nonlinearity parameter takes a positive sign, which is not shown in the figure. $W_0(t)$ in the nonlinear disordered lattice for the nonlinearity parameter outside the self-trapping range is less than that in the linear one at the same time instant, indicating that the off-diagonal nonlinearity to some extent reduces the localization of the wave packet. When v_n is located within the self-trapping interval, $W_0(t)$ is always quite large, i.e., the nonlinearity effect dominates in this case; the only effect of diagonal disorder is to broaden the probability distribution.

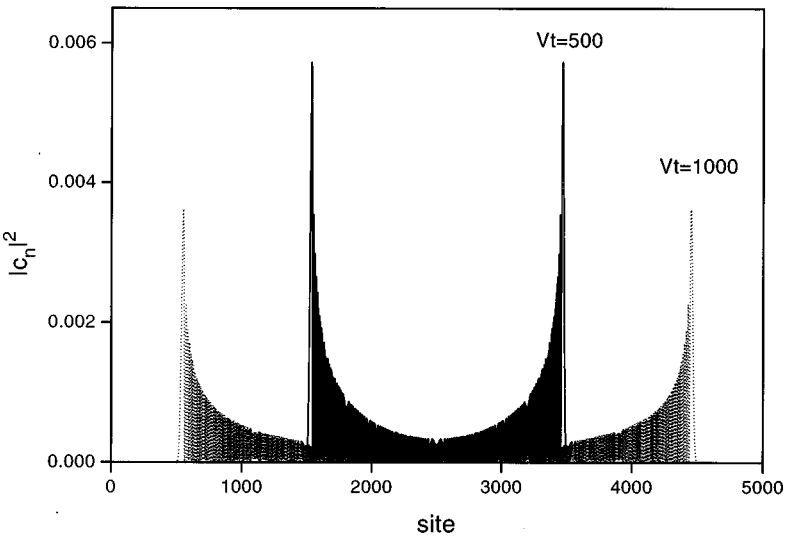

FIG. 9. The spatial distribution of a wave packet for a periodic lattice with fixed nonlinearity parameter $v_n=-0.8V$ at different time instants.

Figure 6 gives the root-mean-square displacement for different nonlinearity parameters. We can see that $\Delta n(t)$ grows rapidly with time at first, indicating an initial expansion of the wave packet, and after some time the growth becomes very slow. The wave packet is still localized in this case. However, $\Delta n(t)$ is larger for larger nonlinearity parameters, indicating that the wave packet is less localized in the off-diagonal nonlinear lattice than in the linear one. By fitting the curves, we find that γ in Eq. (8) is 0 in this case, while in the disordered lattice with diagonal nonlinearity $\gamma=\frac{1}{5}$.

Figure 7 shows the time dependence of the participation number. It oscillates quickly and is not unlimited. We see that the participation number is quite small compared to the lattice length. In the nonlinear disordered case, the participation number is larger than that in the linear disordered case, indicating that off-diagonal nonlinearity can to some extent enhance the width of wave packet.

In order to show more clearly the configuration of wave packet, we demonstrate the spatial distribution of the wave packet in Figs. 8 and 9. In Fig. 8 we show the spatial distribution of the wave packet at different time instants for a given nonlinearity parameter $v_n=-0.9V$. We can see that the spatial distribution changes little with time. The only effect of the off-diagonal nonlinearity is that the wave amplitude at the initial site is smaller than that in the linear lattice at the same time instant. The width of the wave packet is broadened due to off-diagonal nonlinearity. As a comparison we plot the spatial distribution of the wave packet of the MNLSE in a nonlinear periodic lattice in Fig. 9. There are two peaks at the two ends of the wave packet, and the distribution is under an envelope curve. This distribution in the nonlinear periodic lattice is similar to the result of that in the linear periodic lattice [23] since the wave packet propagates ballistically in the nonlinear lattice just as in linear one.

V. SUMMARY

The dynamical properties of the MNLSE have been investigated by studying the time evolution of wave packet in periodic and disordered lattice for different nonlinearity parameters. In the periodic lattice we find an interesting self-trapping phenomenon that occurs only in a narrow interval of the nonlinearity parameter, which is different from the results of diagonal nonlinearity, where self-trapping always occurs if the nonlinearity parameter is greater than a critical value. According to our results, the self-trapping occurs when v_n is negative and $|v_n|$ lies in the interval $(V,1.4V)$. The wave packet propagates ballistically in the MNLSE in a periodic lattice. When self-trapping occurs, the wave packet propagates ballistically at a rate less than that of the untrapping case. Contrary to the results of the diagonal nonlinearity case, the propagation velocity of a wave packet in the MNLSE is greater than that in a linear lattice, and it increases with the increase of the nonlinearity parameter. Thus off-diagonal nonlinearity can help to enhance the propagation of an initially localized mode in a periodic lattice. As for the combined effects of off-diagonal nonlinearity and diagonal disorder on localization, we find that off-diagonal nonlinearity cannot destroy localization as diagonal nonlinearity does. The existence of off-diagonal nonlinearity only slightly expands the localized wave packet.

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