Thermal enhancement and stochastic resonance of polaron ratchets

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(Received 17 March 2014; published 9 June 2014)

We study the ratchet drift of large polarons (solitons) in molecular diatomic chains induced by unbiased time periodic electric fields at nonzero temperature below its critical value. We show that, at a nonzero temperature, the critical value of the intensity of the electric field above which the ratchet phenomenon takes place is lower than at zero temperature for the same frequency of the field. We show that there is a range of temperatures for which the polaron drift is larger than that at zero temperature. We also show that temperature decreases the value of the lowest critical period of the field. And, finally, we demonstrate that there is a stochastic resonance in a polaron ratchet, namely that there is an optimal temperature at which the polaron drift is a maximum. The values of the stochastic resonance temperature, the lowest critical values of the field intensity, and its period depend on various parameters of the system and, in particular, on the anisotropy of the chain parameters. This temperature induced decrease of the critical value of the field intensity and its period, as well as the stochastic resonance itself, may be important for practical applications of the ratchet phenomenon in systems involving conducting polymers and other low-dimensional materials. They may also be important in some biological macromolecules where the ratchet phenomenon could take place in biomotors and energy and/or charge transport.

DOI: 10.1103/PhysRevE.89.062905 PACS number(s): 05.45.−a, 71.38.−k, 63.20.kd, 05.40.−a

I. INTRODUCTION

Low-dimensional molecular systems such as conducting polymers, macromolecules, and others are of great practical importance and are widely used in microelectronics and nanotechnologies because of their special physical properties, one of which is their unusually high conductivity, which can be explained in terms of the large polaron mechanism.

For some of these systems the physical parameters take their values in the range in which their relevant equations can be obtained within the adiabatic approximation. In some of them the values of the electron-phonon coupling and of the nonadiabaticity parameter are just such that they lead to the formation of a large polaron state which, in quasi-one-dimensional systems, is called the "molecular soliton."

Such a soliton describes a quasiparticle (exciton, electron, or hole), which extends over a few lattice sites and is self-trapped in a solitonlike state due to its binding to the local distortions of the lattice [1–5]. A few years ago it was shown theoretically that an external nonbiased (zero mean) periodic field, under certain conditions, can induce a drift of charged solitons [6–9]. This phenomenon, known as the ratchet behavior [10], has been attracting a great deal of attention due to its importance both for the understanding of the functioning of biological motors [11–16] and for promising technical applications in nanotechnologies, including molecular motors. Hence, as a result of many studies, the fundamentals of the ratchet phenomenon are now well understood and many interesting theoretical models of ratchets have been proposed. Moreover, a large variety of experimental realizations have become available (for a review see, e.g., [10] and references therein).

In general, the necessary conditions for the ratchet phenomenon induced by external forces, both in classical and quantum systems, involve energy dissipation in the system and the breaking of possible spatial and/or temporal symmetries of the system [10,17]. The mechanism responsible for the appearance of a directed motion caused by a zero-mean force has been well understood for particles moving in spatial periodic potentials, such as particle separating devices [18] and relativistic particles [19]. Relatively recently ratchet dynamics has been shown to exist for quasiparticles, such as solitons and large polarons [6–9,20–23]. In particular, it has been demonstrated that directed transport of bright solitons formed in a quasi-one-dimensional nondissipative Bose-Einstein condensate can be induced by a weak spatiotemporal biharmonic optical lattice potential [24–27].

Furthermore, it has been shown [10] that the ratchet phenomenon in some systems can also arise due to the action of not only deterministic but also stochastic unbiased time periodic forces (ac), such as temporal [10], spatial [28], and quenched temporal [29] disorder. In most cases these studies were performed for the case of zero temperature, although it has been shown that solitons can exhibit ratchet behavior at nonzero temperatures as well [30].

As mentioned above, the ratchet mechanism at zero temperature in (quasi-)one-dimensional molecular chains, which supports the existence of electron self-trapped states, was studied in Refs. [6–9]. These papers have shown that the phenomenon arises due to the presence of the Peierls-Nabarro potential barrier and that it takes place only when the intensity of the field and its period are sufficiently large (i.e., there exist critical values of these quantities below which the effect does

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not take place). Hence it is natural to ask if such solitons can exist and drift, in nonbiased ac electric fields, also at nonzero temperatures.

Hence in this paper we study the ratchet behavior of charged polarons (electrosolitons) in thermalized anisotropic molecular chains and, in particular, chains which in their unit cell contain two different atoms. We show that under certain conditions the thermal noise not only does not prevent the drift of polarons but that it even generates it at a lower critical value of the intensity of the field than at zero temperature. We also show that the lower critical value of the period of the electric field decreases with the increase of the temperature. Moreover, our numerical results demonstrate the existence of a stochastic resonance in the polaron drift, namely, that the amplitude of the polaron drift has a nonmonotonic dependence on temperature, described by a characteristic Λ-shaped curve.

It is worth mentioning here that the thermal fluctuations modify the properties of the solitons and, when the temperature is sufficiently high, they can even destroy them: as the thermal oscillations of the lattice become too strong, the electron (hole) cannot remain bound with the self-induced local lattice distortions and, as a consequence, the polaron is unstable and decays into an unbound delocalized state. So our study was restricted to temperatures for which the polaron was stable.

II. HAMILTONIAN OF THE SYSTEM AND DYNAMICAL EQUATIONS

To study the ratchet phenomenon for molecular solitons, we consider an extra electron in a diatomic molecular chain, in the nearest-neighbor approximation and in the presence of an external periodic unbiased electromagnetic field at nonzero temperature. The states of an extra electron in such a system are described by the Fröhlich Hamiltonian which can be written as a sum of three terms:

$$H = H_{ph} + H_e + H_{e\text{-}ph}. \tag{1}$$

Here H_{ph} is the Hamiltonian of the lattice vibrations, H_e is the electron Hamiltonian, and $H_{e\text{-}ph}$ describes the electron-phonon interaction. For the numerical simulations it is convenient to use each of these Hamiltonians in the site representation.

Let $z^0_{n,1} = na$, $z^0_{n,2} = na + b$ denote the equilibrium positions of two different atoms, or groups of atoms, per unit cell, periodically arranged along the chain axis, with a being the lattice constant and b being the distance between the two atoms in one unit cell.

The Hamiltonian of the lattice vibrations, H_{ph}, in the harmonic approximation is given by

$$H_{ph} = \frac{1}{2}\sum_n \left[\frac{p^2_{n,1}}{M_1} + \frac{p^2_{n,2}}{M_2} + w_s(u_{n,1} - u_{n,2})^2 + w_l(u_{n,1} - u_{n-1,2})^2 \right], \tag{2}$$

where M_1 and M_2 are masses of atoms, $u_{n,j}$ are longitudinal displacements of atoms from their equilibrium positions, $z_{n,j} = z^0_{n,j} + u_{n,j}$, and $p_{n,j}$ are the momenta, canonically conjugate to $u_{n,j}$. Finally, w_s and w_l are the elasticity constants describing the strengths of the interactions between the nearest-neighbor atoms belonging to, respectively, the same cell and to the neighboring cells.

Introducing creation and annihilation operators of an electron on the site (n, j), $a^\dagger_{n,j}$, $a_{n,j}$, the electron Hamiltonian can be written as

$$H_e = \sum_n [\mathcal{E}_1\, a^\dagger_{n,1} a_{n,1} + \mathcal{E}_2\, a^\dagger_{n,2} a_{n,2} - J_s(a^\dagger_{n,1} a_{n,2} + a^\dagger_{n,2} a_{n,1}) - J_l(a^\dagger_{n,1} a_{n-1,2} + a^\dagger_{n-1,2} a_{n,1})], \tag{3}$$

where $\mathcal{E}_j$ is the on-site electron energy which includes also the influence of the neighboring atoms; J_s and J_l are the resonant (exchange) energies of an electron on the nearest neighbors from the same unit cell and from the neighboring cells, respectively.

The electron-phonon interaction describes the dependence of the exchange interaction energies J_s, J_l and of the on-site energy $\mathcal{E}_j$ on the interatomic separation. Taking into account such a dependence of the on-site energy only, we obtain the electron-phonon interaction Hamiltonian, $H_{e\text{-}ph}$, which, in the linear approximation with respect to the lattice displacements, takes the form

$$H_{e\text{-}ph} = \sum_n [\, a^\dagger_{n,1} a_{n,1}\, [\chi_l\,(u_{n,1} - u_{n-1,2}) + \chi_s\,(u_{n,2} - u_{n,1})] + a^\dagger_{n,2} a_{n,2}\, [\chi_l\,(u_{n+1,1} - u_{n,2}) + \chi_s\,(u_{n,2} - u_{n,1})]]. \tag{4}$$

Here χ_s and χ_l are the coefficients of the electron-phonon interaction between the nearest neighbors belonging to, respectively, the same unit cell and to the neighboring cells.

Diagonalizing the electron and phonon Hamiltonians (3) and (2), we find that in such a chain there are two electron bands and two phonon modes. The dispersion laws $E_\lambda(q)$ of the two electronic bands, labeled by the index $\lambda = U, L$ for the upper and lower ones, are

$$E_\lambda(q) = \mathcal{E}_0 \pm \frac{1}{2}\sqrt{\Delta_0^2 + 4J^2 - 16 J_s J_l \sin^2\frac{qa}{2}}. \tag{5}$$

The frequencies of the two phonon modes, acoustical (ac) and optical (op), are given by

$$\omega^2(q) = \frac{1}{2}\left(\frac{W}{\mu} + \epsilon_{\text{mode}} \sqrt{\frac{W^2}{\mu^2} - 16\frac{w_s w_l}{M_1 M_2}\sin^2\frac{qa}{2}} \right). \tag{6}$$

where $\epsilon_{\text{ac}} = -1$ and $\epsilon_{\text{op}} = 1$. Here $q = \frac{2\pi}{Na}\nu$ ($\nu = 0, \pm 1, \dots$) denotes the quasimomentum, and we have introduced the following notation: $\mathcal{E}_0 = (\mathcal{E}_2 + \mathcal{E}_1)/2$, $\Delta_0 = \mathcal{E}_2 - \mathcal{E}_1$, $J = J_s + J_l$ and $\mu = M_1 M_2/M$, $M = M_1 + M_2$, $W = w_s + w_l$.

Self-trapped states of electrons correspond to the energy ground states in molecular systems which satisfy the conditions of the adiabatic approximation. This approximation is equivalent to the semiclassical considerations in which the lattice subsystem can be treated as a classical one. In the adiabatic approximation the wave function of the system is represented in a multiplicative Born-Oppenheimer form which, for one extra electron in the chain, takes the form

$$|\Psi\rangle = U\,|\psi_e\rangle, \quad |\psi_e\rangle = \sum_{n,j} \Psi_{n,j} a^\dagger_{n,j}|0\rangle, \quad j = 1,2, \tag{7}$$

where U is the unitary operator of the coherent displacements of atoms induced by the presence of an electron in the state $|\psi_e\rangle$. Here $|0\rangle$ denotes the corresponding vacuum state and $\Psi_{n,j}$ is the electron wave function, normalized to unity.

One can then easily compute the Hamiltonian function $\mathcal{H} = \langle\Psi|H|\Psi\rangle$:

$$\begin{aligned}\mathcal{H} = \sum_n \Big[& \mathcal{E}_1|\Psi_{n,1}|^2 + \mathcal{E}_2|\Psi_{n,2}|^2 - (J_s\Psi_{n,1}\Psi^*_{n,2} + J_l\Psi_{n,1}\Psi^*_{n-1,2} + \text{c.c.}) + \frac{1}{2}\Big[\frac{p^2_{n,1}}{M_1} + \frac{p^2_{n,2}}{M_2} + w_s(u_{n,1}-u_{n,2})^2 \\ & + w_l(u_{n,1}-u_{n-1,2})^2\Big] + \chi_l\,[|\Psi_{n,1}|^2(u_{n,1}-u_{n-1,2}) + |\Psi_{n,2}|^2(u_{n+1,1}-u_{n,2})] \\ & + \chi_s\,[|\Psi_{n,1}|^2(u_{n,2}-u_{n,1}) + |\Psi_{n,2}|^2(u_{n,2}-u_{n,1})]\Big]. \end{aligned} \tag{8}$$

From the Hamiltonian function (8) we obtain a system of coupled dynamical equations for the electron and lattice variables $u_{n,l}$ and $\Psi_{n,l}$ and their conjugated momenta.

For numerical simulations it is convenient to use dimensionless units; thus, we introduce time measured in units of $\hbar/J$, energy measured in units of J, and displacements measured in units of length $l = \hbar\sqrt{2/JM}$. We also introduce the dimensionless parameters m, w, d, and x by the relations

$$\begin{aligned} M_{1,2} &= \tfrac{1}{2}M(1\pm m), \quad w_{s,l} = \tfrac{1}{2}W(1\pm w), \\ J_{s,l} &= \tfrac{1}{2}J(1\pm d), \quad \chi_{s,l} = \tfrac{1}{2}X(1\pm x), \end{aligned} \tag{9}$$

or, respectively,

$$\begin{aligned} m &= \frac{M_1-M_2}{M}, \quad w = \frac{w_s-w_l}{W}, \quad d = \frac{J_s-J_l}{J}, \\ x &= \frac{\chi_s-\chi_l}{X}, \quad X = \chi_s+\chi_l. \end{aligned} \tag{10}$$

To study the ratchet phenomenon induced by the electromagnetic oscillating field, $E(t)$, in a thermalized diatomic chain we have to include in the corresponding equations terms describing the interaction of the system with the external field, the presence of the energy dissipation in the system, as well as terms describing the thermal fluctuations of the lattice. Therefore, we add the term $E(t)(n-n_0)\Psi_{n,l}$ to the equation for $\Psi_{n,l}$ to describe the action of the electric field. We also add the terms $F(t) - \Gamma\frac{du_{n,j}}{dt}$ to the equations for $u_{n,j}$ where the first one is a Langevin factor describing thermal excitations (it is discussed below), and the second one describes the energy dissipation due to viscous friction where Γ is the friction coefficient.

As a result, in these dimensionless units, the dynamical equations for such a system at nonzero temperature in the external electric field take the following form:

$$\begin{aligned} i\frac{d\Psi_{n,1}}{dt} &= \Big[-1+\frac{D}{2}+E(t)(n-n_0)\Big]\Psi_{n,1} + \frac{1}{2}(1+d)\Psi_{n,2} + \frac{1}{2}(1-d)\Psi_{n-1,2} \\ &\quad + G[(1+x)(u_{n,1}-u_{n,2}) - (1-x)(u_{n,1}-u_{n-1,2})]\Psi_{n,1}, \\ i\frac{d\Psi_{n,2}}{dt} &= \Big[-1-\frac{D}{2}+E\Big(n-n_0+\frac{b}{a}\Big)\Big]\Psi_{n,2} + \frac{1}{2}(1+d)\Psi_{n,1} + \frac{1}{2}(1-d)\Psi_{n+1,1} \\ &\quad + G[(1+x)(u_{n,1}-u_{n,2}) - (1-x)(u_{n+1,1}-u_{n,2})]\Psi_{n,2}, \\ \frac{d^2u_{n,1}}{dt^2} &= -\frac{C}{1-m}[(1+w)(u_{n,1}-u_{n,2}) + (1-w)(u_{n,1}-u_{n-1,2})] \\ &\quad + \frac{G}{1-m}[2x|\Psi_{n,1}|^2 - (1-x)|\Psi_{n-1,2}|^2 + (1+x)|\Psi_{n,2}|^2] + F_{n,1}(t) - \Gamma\frac{du_{n,1}}{dt}, \\ \frac{d^2u_{n,2}}{dt^2} &= \frac{C}{1+m}[(1+w)(u_{n,1}-u_{n,2}) + (1-w)(u_{n+1,1}-u_{n,2})] \\ &\quad + \frac{G}{1+m}[-2x|\Psi_{n,2}|^2 + (1-x)|\Psi_{n+1,1}|^2 - (1+x)|\Psi_{n,1}|^2] + F_{n,2}(t) - \Gamma\frac{du_{n,2}}{dt}. \end{aligned} \tag{11}$$

Here the intensity of the electric field $E(t)$ is measured in units ea/J and we have further defined

$$G = \frac{Xl}{2J}, \quad C = \frac{\hbar^2 W}{MJ^2}, \quad D = \frac{\mathcal{E}_2-\mathcal{E}_1}{J}, \quad k = \frac{k_B}{J}, \tag{12}$$

where k_B is the Boltzmann structure constant (so that kT denotes thermal energy in units of J).

The thermal noise $F(t)$ can be taken as a Gaussian white noise of zero mean value and variance given by

$$\langle F_{n,i}(t_1)F_{m,j}(t_2)\rangle = 2\Gamma kT\delta(t_1-t_2)\delta_{n,m}\delta_{i,j}, \tag{13}$$

i.e., we describe it by a random function with a normal distribution satisfying the constraint (13). In our numerical

simulations $F(s)$ is constant during the time step interval dt and $\delta(t_2 - t_1) = 1/dt$.

III. RATCHET PHENOMENON IN ASYMMETRIC CHAINS

First of all, let us recall that the existence of the polaron ratchet behavior is due to the Peierls-Nabarro barrier experienced by the polaron propagating on a discrete lattice [31–34] as this barrier, for asymmetric diatomic lattices, is spatially asymmetric [9], and so this periodic asymmetric potential plays the role of the ratchet potential.

We have verified this by performing several sets of numerical simulations for various values of the anisotropy parameters. From our previous studies [6] we know that the dynamics of the polaron is very complex even at zero temperature. Hence, in our new studies we have, to begin with, taken as nonzero only one anisotropy parameter with the others being set equal to zero. After analyzing the obtained results, we performed simulations with two or all of them being nonzero. The results of these simulations are discussed below.

To study the dynamics of an electron in a chain subjected to thermal fluctuations, we started by computing numerically a stationary solution of Eqs. (11), at zero temperature, in the absence of an external field, i.e., by setting $E(t) = 0, kT = 0$. Then we used this obtained solution as the initial condition for a numerical integration of Eqs. (11) when the electric field $E(t)$ was not zero. All our numerical simulations were performed for a chain of 200 nodes.

In this paper we first present the results obtained for the parameter values $G = 0.4$, $C = 0.22$, $D = 0.1$, $\Gamma = 0.2$, and $m = 0$. This choice of values was dictated by wanting to be close to the realistic parameter values for the α-helical proteins and they correspond to the values at which the polaron is neither too narrow, nor too broad. For these parameters values, the stationary solutions are self-trapped within a few lattice sites. When the temperature is nonzero, the same simulation produces a different drift for each run because of the built-in stochasticity of the temperature effects. All the results presented in this paper were obtained by performing 100 simulations, except for $kT = 0$ for which we only performed one, for each set of parameters and then computing the average values of the resultant drifts. As in Ref. [6] the drifts were measured as the average drift per period or, in other words, the total polaron displacement during a time interval t divided by the number of periods t/T_e.

In Ref. [6] we showed that the asymmetry parameters m and D do not induce a ratchet effect, so in our studies we have only varied the values of the anisotropy parameters x, d, and w. As we showed in Refs. [6,8] that in anisotropic chains the ratchet effect can be induced even by a harmonic, i.e., time-symmetric ac field, we have chosen the electric field to be of the form $E(t) = E_0 \sin(2\pi t/T_e)$.

We have also shown in Refs. [6,8] that for the ratchet effect to take place the intensity of the field and its period have to exceed some critical values, $E_0 > E_{cr}$, $T_e > T_{e,cr}$. If the period of the external force is below this value the frequency of the polaron oscillations within the potential well of the Peierls-Nabarro barrier is high and the amplitude of the polaron oscillations that are caused by the oscillating external field is small. Thus, $A \propto E_0 T_e^2 \ll a$ and the polaron cannot overcome the intersite distance and remains pinned, i.e., under such conditions the polaron cannot drift.

To determine the polaron drift as a function of the intensity of the field, we have chosen a period of the field sufficiently large so that the lattice deformation could follow the oscillations of the electron, caused by the periodic force. Thus, we have chosen $T_e = 1000$.

A. Polaron drift

We have started our investigations by studying the temperature dependence of the ratchet effect when the electron-phonon coupling is not symmetric, i.e., when x is nonzero.

In Fig. 1(a) we present the amplitude of the polaron drift, as a function of the intensity of the field, for the chain at $x = 0.1$, $d = w = 0.0$ and for several values of the temperature. The amplitude of the drift denotes here the number of lattice sites, at which the center of the polaron shifts within one period of the ac force, i.e., the drift of the polaron per period of the field.

To discuss our results we note, first of all, that they clearly demonstrate that the ratchet behavior of polarons takes place also at nonzero temperatures. As could be expected, there is a critical value of the intensity of the field below which the polaron cannot drift. We have run simulations for several other temperatures and in Table I we present the lowest value of E_0 for which the average drift per period is equal to 0.5, i.e., a displacement of one atom, and 1, i.e., a displacement of two atoms, for various temperatures.

At zero temperature, and for the period of the field mentioned above, the critical value of the field is $E_{0,cr} = 0.092$. When the intensity of the field increases, the amplitude of the drift increases too. However, when the field is too strong, the polaron begins to move so fast that it radiates sound waves very intensively. This leads to the increase of the effective mass of the polaron and these two effects make the drift less regular and weaker; i.e., the amplitude of the drift begins to decrease. Above some upper critical value of the field, $E_0 > E_{cr,2}$, the polaron is destroyed—the electron undergoes a transition from the self-trapped state into a delocalized one. In this paper we have considered a single value of the dissipation parameter Γ. In stronger fields the energy dissipation increases as well, and as a result the polaron drift occurs up to larger values of the electric field. Moreover, at large enough polaron velocities the harmonic approximation in the lattice description ceases to be valid and one has to take into account also the lattice anharmonicity.

When $T \neq 0$ we see straight-away that the first critical value ($E_{0,cr}$) of the field is lower; the polaron drift arises at smaller values of the field intensity and the larger the temperature, the smaller the value of E_{cr}. Thus, $E_{cr}(kT = 0) \approx 0.09$, $E_{cr}(kT = 0.001) \approx 0.06$, and $E_{cr}(kT = 0.002) \approx 0.03$. So at $kT = 0.002$, E_{cr} is only a third of its value at $T = 0$.

When $T = 0$, the maximum average drift per period obtained is four unit cells (eight atoms), and this occurs when $E_0 \approx 0.113$. For this value of E_0, the average drift at nonzero temperatures is smaller (about 2 for $kT = 0.001$ and 1.5 for $kT = 0.002$). Nevertheless, below this field intensity the polaron drift at nonzero temperatures is larger than at $T = 0$.

From Fig. 1(a) we see the nonmonotonic dependence of the polaron drift amplitude on the field intensity. At first,

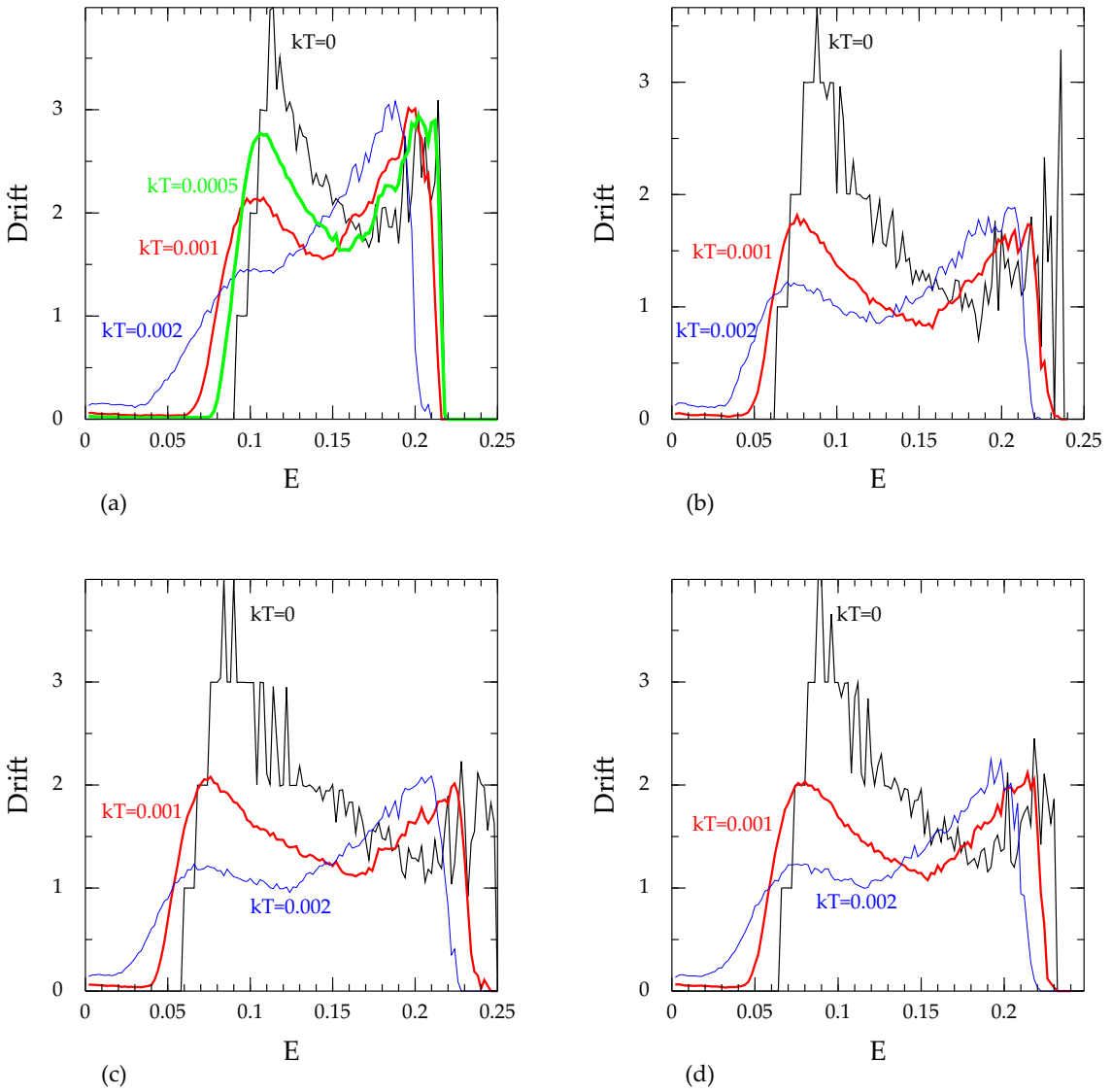

FIG. 1. (Color online) Amplitude of the average polaron drift per period, for several values of the temperature, as a function of the intensity of the electric field with period $T_e = 1000$. Parameter values: (a) $x = 0.1$, $d = w = 0$, $C = 0.22$, $b = 0.5$, $D = 0.1$, $G = 0.4$, $\Gamma = 0.2$; (b) $d = 0.1$, $x = w = 0$, $C = 0.22$, $b = 0.5$, $D = 0.1$, $G = 0.4$; (c) $w = -0.1$, $x = d = 0$, $C = 0.22$, $b = 0.5$, $D = 0.1$, $G = 0.4$; (d) $x = d = -w = 0.03$, $C = 0.22$, $b = 0.5$, $D = 0.1$, $G = 0.4$.

the drift increases with the increase of the field, until it reaches its maximum value at a certain "optimal" intensity of the field. At larger values of the field it decreases due to the stronger radiation of sound waves by the polaron up to the field values at which the corresponding polaron velocity becomes so small that the polaron again begins to increase its drift velocity. At even stronger fields the polaron becomes unstable and decays into a delocalized state. Such nonmonotonic behavior of the polaron drift results from the interplay of the polaron oscillations due to the Peierls-Nabarro potential barrier and those due to the external periodic force. This process depends also on the thermal vibrations of the lattice. When these vibrations become sufficiently strong the deformation potential well gets "wiped out" and, from a certain value of the temperature, the polaron drift smoothly increases with the increase of the field intensity. In the

TABLE I. Smallest electric field intensity, $E_{0,\min}$, for which the average drift per period is 0.5 lattice site (i.e., one atom, top row) or one lattice site (i.e., two atoms, bottom row), for various temperatures. Parameter values: $x = 0.1$, $d = w = 0$, $C = 0.22$, $b = 0.5$, $D = 0.1$, $G = 0.4$, $\Gamma = 0.2$ for an electric field with period $T_e = 1000$.

kT	0	0.0001	0.0002	0.0005	0.0008	0.001	0.0012	0.0015	0.002
$E_{0,\min}(\text{drift} = 0.5)$	0.092	0.09	0.088	0.085	0.078	0.074	0.07	0.063	0.055
$E_{0,\min}(\text{drift} = 1)$	0.092	0.094	0.092	0.088	0.082	0.079	0.076	0.074	0.072

case considered above this takes place around $kT = 0.002$ (see Fig. 1).

At the same time, with the increase of the temperature, the upper critical value of the field decreases. This is due to the fact that with the increase of the polaron velocity and the increase of the thermal fluctuations of the lattice the effective mass of the polaron becomes so large that the bound state of the electron and of the lattice deformation becomes unstable.

It is important to add here that the nonmonotonic dependence of the polaron drift on the intensity of the field changes qualitatively with the increase of the temperature: at low fields the higher the temperature, the stronger the drift. At stronger fields this dependence is reversed: the lower the temperature the stronger the drift, and at even stronger fields this dependence is altered again with the stronger drift resulting from higher temperatures. Similar nonmonotonic dependence of the drift on the field intensity and temperature has also been observed for other cases of the anisotropy parameters, as is discussed below.

We have also observed that when the temperature is too high, the polaron is unstable and the electron becomes delocalized before starting to drift.[1]

Next we have considered the effect of an anisotropy of the exchange interaction energy, i.e., $d \neq 0$. In Fig. 1(b) we present the plots of the amplitude of the polaron drift per period as a function of the intensity of the field for several temperatures when $d = 0.1$ and $x = w = 0$. We see that this anisotropy leads to the appearance of a polaron drift above the critical value of the field $E_{cr}(T = 0) = 0.062$ and that this critical value also decreases with the increase of the temperature: $E_{cr}(kT = 0.001) \approx 0.045$, and $E_{cr}(kT = 0.002) \approx 0.03$. On the other hand, the maximum drift obtained in this class of cases was found to be 3.7 and this was achieved for $T = 0$ at $E_0 \approx 0.088$. Again, the average drift decreases with the increase of kT for that field; i.e., it is 1.6 for $kT = 0.001$ and 1.2 for $kT = 0.002$. From Fig. 1(b) we see also that there is an interval of the temperature values at which, for certain intensities of the field, the drift is stronger than at $T = 0$. We also observe that the amplitude of the electric field at which the electron becomes delocalized decreases with the increase of the temperature.

Finally, we have also observed a ratchet effect when the elasticity coefficient was asymmetric, i.e., at $w \neq 0$. This time, with our definition of w, when $w > 0$ the polaron drifts in the opposite direction. For this reason, we report here the results for the value $w = -0.1$ so that we can more easily compare the figures for the different cases. This is shown in Fig. 1(c) and we notice that $E_{cr}(T = 0) = 0.058$, $E_{cr}(kT = 0.001) \approx 0.04$, and $E_{cr}(kT = 0.002) \approx 0.02$. Again, we see that in the relatively weak fields the maximum drift is stronger, at not-too-high nonzero temperatures, than at $T = 0$. For the value of $E = 0.078$ the drift at $kT = 0.001$ is stronger than at $kT = 0$. We also notice that the electric field amplitude at which the electron becomes delocalized decreases as the temperature increases.

[1]The thermal stability of the polaron in our and other, more physical, systems will be analyzed in more detail and discussed in a future publication.

We have also studied the case of all three anisotropies x, d, and w being nonzero simultaneously and we have considered the case of $x = d = -w = 0.03$. We have taken this smaller value because the anisotropies tend to increase the depth of the well in which the polaron is trapped and so make the drift harder to take place. The results are presented in Fig. 1(d). We note that the results qualitatively are similar to those of the previous cases; this time we have $E_{cr}(T = 0) = 0.066$, $E_{cr}(kT = 0.001) \approx 0.045$, and $E_{cr}(kT = 0.002) \approx 0.03$.

B. Polaron trajectories

We have also analyzed in detail the trajectories followed by individual polarons. When the electric field is too low, $E < E_{cr}$, the polaron is pinned by the lattice and wobbles inside the lattice's cell, as shown in Fig. 2(a); see the curve for $kT = 0$. When the electric field is just above its critical value, the polaron moves in steps, as shown in Fig. 2(b). When the electric field becomes larger, the polaron starts to drift: it moves forward by several lattice sites and then moves backward by a smaller amount, hence moving effectively by one or more lattice sites during each period (see [6] for a detailed analysis).

When the temperature is nonzero, the behavior remains essentially the same, except that the trajectory exhibits also some randomness due to the thermal noise. We have also noticed that, as the temperature increases, the amplitude of the polaron oscillations increases. This is clear from Fig. 2(b), which shows that an increase of temperature, up to a certain value, results in the increase of the polaron drift (compare the curves for $kT = 0$ and $kT = 0.001$). With a further increase of the temperature, oscillations of the polaron become stronger, its effective mass becomes larger, and the polaron drift decreases and becomes smaller than at $T = 0$. In Fig. 2(c) we show the position of the polaron over 800 full periods of the electric field for $kT = 0$, $kT = 0.0005$, and $kT = 0.001$. One clearly sees that the polaron oscillates as it jumps between lattice sites but that it also exhibits a random motion over long distances when the temperature is nonzero.

IV. STOCHASTIC RESONANCE OF THE POLARON DRIFT

In this section we analyze the effects of the temperature on the dependence of the polaron drift as one varies the period of oscillations of the electric field. It is worth recalling that at zero temperature there is a critical value of the period of the oscillating field below which there is no drift of polarons. This is because, in a lattice, the periodic Peierls-Nabarro barrier plays the role of the ratchet potential. This barrier itself, even in the absence of the external periodic force, results in the oscillating character of the polaron velocity. In the presence of the oscillating external force these oscillations add up to the force induced oscillations with the frequency of the external field. At low frequencies an electron and self-induced lattice deformation oscillate together in a bound polaron state. If the frequency of the field is very high, the local deformation of the chain cannot follow fast oscillations of the electron, and so the electron does not feel the Peierls-Nabarro potential. Therefore, at high frequencies of the field the necessary conditions for the existence of the ratchet phenomenon become violated.

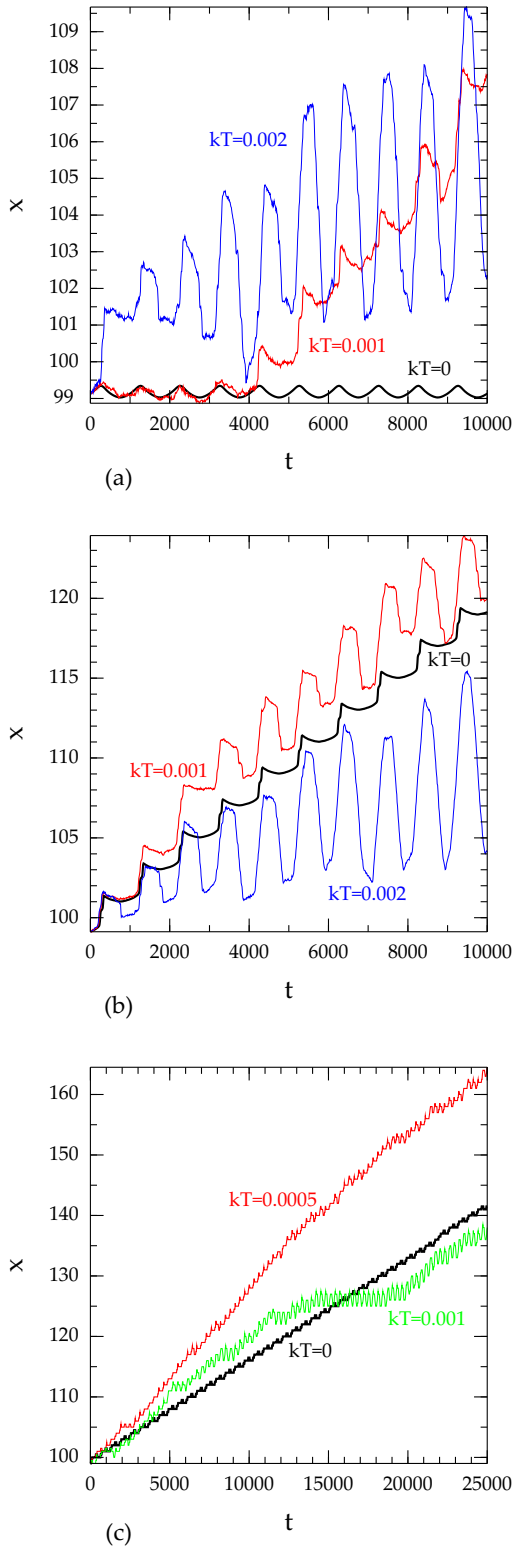

FIG. 2. (Color online) Position of the polaron as a function of time for (a) $E = 0.08$, $T_e = 1000$; (b) $E = 0.1$, $T_e = 1000$; and (c) $E = 0.1$, $T_e = 300$ at different temperature. Parameter values: $x = 0.1$, $d = w = 0$, $C = 0.22$, $b = 0.5$, $D = 0.1$, $G = 0.4$, and $\Gamma = 0.2$.

At nonzero temperature thermal vibrations of the lattice lead to the deterministic self-consistent displacements of atoms, creating a periodic potential and, as a result, the critical

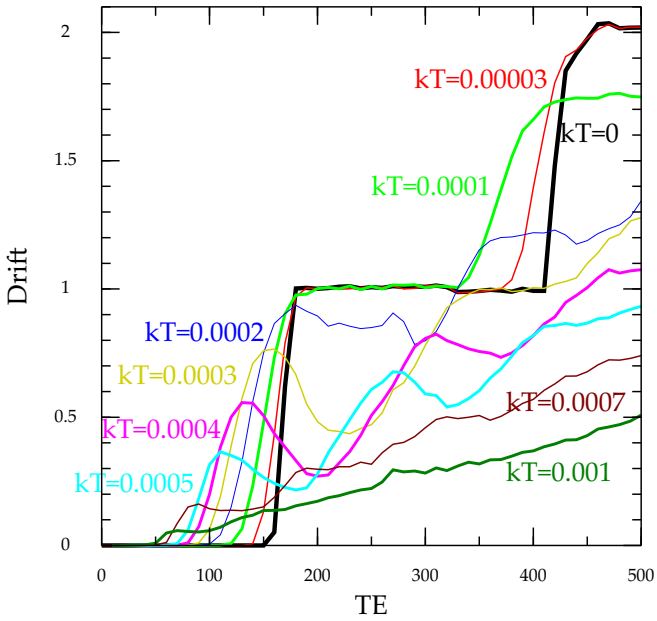

FIG. 3. (Color online) Amplitude of the polaron drift per period as a function of the period of oscillations of the electrical field of the intensity $E_0 = 0.11$ at different temperatures. Parameter values: $x = 0.1, d = w = 0, C = 0.22, b = 0.5, D = 0.1, G = 0.4$, and $\Gamma = 0.2$.

value of the period of the field decreases, and can even disappear, as can be deduced from looking at Fig. 3. From this figure we can also conclude that the amplitude of the drift has a nonmonotonic dependence on the period of the field within a certain interval of temperatures. This indirectly indicates the possibility of the existence of a stochastic resonance in the polaron drift.

To study this in detail, we performed two sets of numerical simulations for two different values of the intensity of the field for various periods of the field below the corresponding critical value at zero temperature. These results are presented in Fig. 4, which show the nonmonotonic dependence of the amplitude of polaron drift on the temperature with a sharp maximum for an intermediate (finite) value of temperature; i.e., this dependence exhibits a characteristic Λ resonance shape. Namely, for a given set of parameters of the system there exists an optimal temperature at which the drift of a polaron is the largest. The bigger the period of the field, the stronger the drift, and the larger the maximum value of the drift, the lower the optimal temperature. Moreover, at the lower value of the intensity of the field the polaron drift is largest [compare Figs. 4(a) and 4(b)]. We also see in Fig. 4(b) a second maximum of the amplitude of the drift for larger values of the temperature.

We have also investigated the dependence of the drift and the stochastic resonance on the value of the dissipation parameter Γ. For polarons, the range of values of Γ for which the ratchet effect takes place, while maintaining all the other parameters fixed, is restricted by the stability properties of the polaron. For small values of Γ, the polaron is rapidly destroyed by the electric field before any drift can be initiated. When Γ is too large, on the other hand, the polaron can only move for large amplitude of the electric field, so large that the polaron is destroyed too. In Fig. 4(c) we present the average drift per

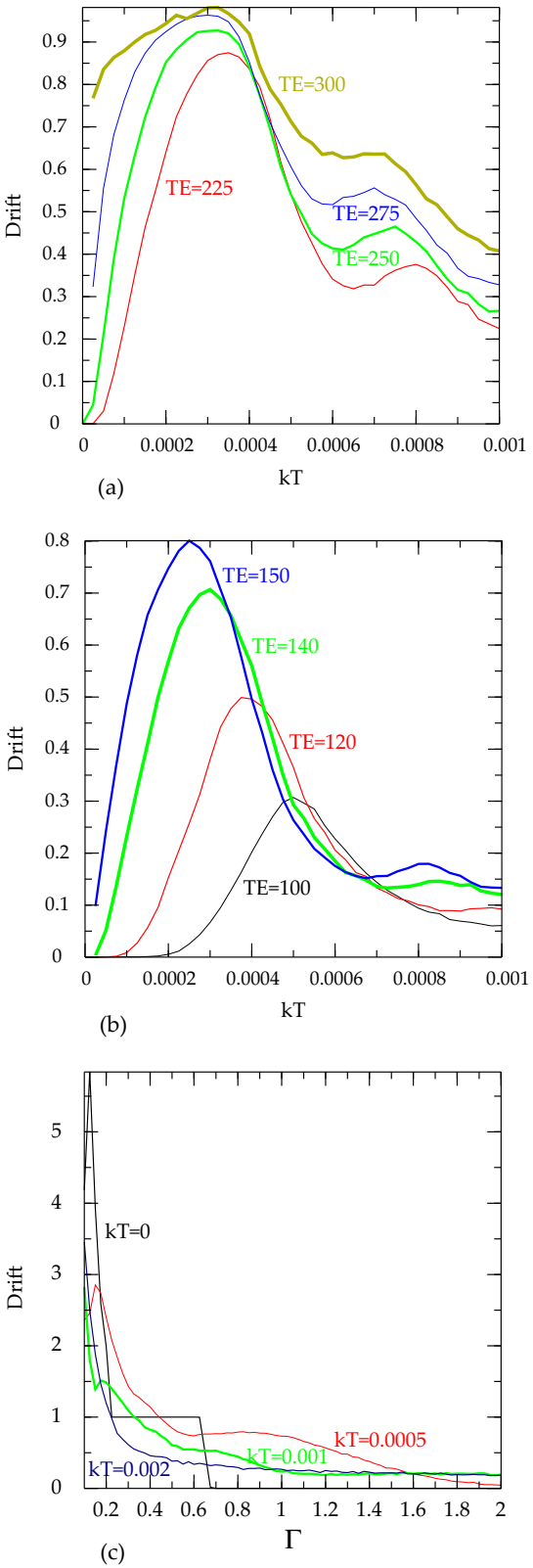

FIG. 4. (Color online) (a),(b) Amplitude of the polaron drift as a function of temperature for different values of the period of the field for $x = 0.1$, $d = w = 0$, $C = 0.22$, $b = 0.5$, $D = 0.1$, $G = 0.4$, and $\Gamma = 0.2$. (a) $E = 0.1$; (b) $E = 0.11$, $T_e = 1000$. (c) Polaron drift as a function of the dissipation parameter Γ for different temperatures. Parameter values: $x = 0.1$, $d = w = 0$, $C = 0.22$, $b = 0.5$, $D = 0.1$, and $G = 0.4$.

period of a polaron as a function of Γ. First of all we see that the drift varies with Γ and that the stochastic resonance occurs for all dissipation values at which the polaron ratchet can be induced. It is worth comparing these results with those of [35,36], where a stochastic resonance was observed for particles trapped in an asymmetric periodic potential. Because particles are intrinsically stable, any value of Γ was allowed, unlike the polaron which can decay rapidly when subjected to large excitations. In the parameter domain where the polaron is stable, our results agree with what was observed in the above-mentioned two papers.

It was also observed [35,36] that for some frequencies and for some values of Γ, the direction of the drift was sometimes reversed. We did not observe this phenomenon in any of our simulations. While this was sometimes seen for individual thermal simulations, when computing the average drift over 100 simulations, at the same temperature, the average drift was always positive or zero.

All these results can be partially understood using the following arguments based on the collective coordinates approximation to the description of the polaron. The stationary polaron solution can be found from the system of Eqs. (11). Let us consider first a diatomic molecular chain with the only nonzero anisotropy parameter, $x \neq 0, d = w = 0$, and $a = 2b$, as considered in the numerical simulations described in this section. From the equations for the lattice displacements, Eqs. (11), we find that

$$\begin{aligned} u_{n,1} - u_{n,2} &= (1+x)\frac{G}{C}(|\Psi_{n,1}|^2 + |\Psi_{n,2}|^2), \\ u_{n-1,2} - u_{n,1} &= (1-x)\frac{G}{C}(|\Psi_{n-1,2}|^2 + |\Psi_{n,1}|^2). \end{aligned} \tag{14}$$

Substituting these expressions into the equations for the electron wave functions in Eqs. (11), we obtain discrete nonlinear Schrödinger equations for $\Psi_{n,1}$ and $\Psi_{n,2}$, whose solution, in the continuum limit, $\Psi_{n,1} = \Psi(\zeta)$, $\Psi_{n,2} \approx \Psi(\zeta) + b\frac{d\Psi}{d\zeta} + \frac{b^2}{2}\frac{d^2\Psi}{d\zeta^2}$, is given by

$$\Psi(\zeta) = \sqrt{\frac{\kappa}{2}}\frac{\exp(-i\mathcal{E}_s t)}{\cosh[\kappa(\zeta - R)]}, \tag{15}$$

where R and $\mathcal{E}_s$ are the center-of-mass coordinate and the eigenenergy of the polaron, respectively, measured in nondimensional units. The inverse width of the polaron is given by the expression

$$\kappa = (1+x^2)\frac{4G^2}{C}. \tag{16}$$

According to [34], in a lattice, a polaron propagates in a periodical Peierls-Nabarro potential. For a diatomic chain this potential can be written in the form

$$U_{\mathrm{PN}} = U_0\left[\cos\left(\frac{\pi R}{b} + \phi_0\right) + \cos\left(\frac{2\pi R}{b} - \phi_0\right)\right]. \tag{17}$$

Here the phase shift $\phi_0 \approx 2x$ describes the asymmetry of the electron-lattice interaction in a diatomic chain, resulting in the relation (14). The amplitude of the Peierls-Nabarro potential, U_0, measured in units of energy J, is determined by the inverse

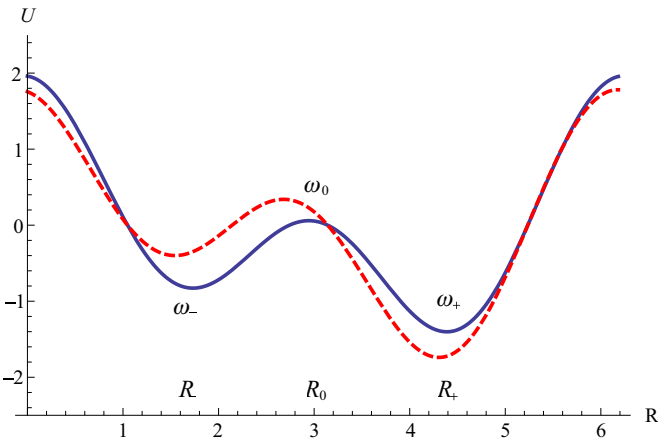

FIG. 5. (Color online) Peierls-Nabarro potential (17) in units of U_0 for $x = 0.1$. R is in units of b/π.

width of the polaron, κ:

$$U_0 = \frac{2(\pi^2+4)}{\kappa} e^{-\frac{\pi^2}{2\kappa}}. \tag{18}$$

Note that the Peierls-Nabarro potential has the form of an asymmetric double-well potential with two minima at

$$R_- \approx \frac{\pi+\phi_0}{2}, \quad R_+ \approx \frac{3\pi+\phi_0}{2} \tag{19}$$

and a local maximum at $R_0 \approx b$, as one can see from Fig. 5.

In the presence of an external oscillating electrical field $E(t)$ and taking into account the energy dissipation, the equation of motion for the center of mass of the soliton R takes the form

$$M_s \frac{d^2R}{dt^2} = -\frac{dU_{\rm PN}}{dR} + E_0 \sin\left(\frac{2\pi t}{T}\right) - \Gamma\frac{dR}{dt} + F(t), \tag{20}$$

where $F(t)$ is a random "force" describing the thermal vibrations of atoms in the lattice, whose properties are described in more detail at the end of Sec. II.

According to the theory of stochastic processes, the dynamics of the system, described by Eq. (20), in the absence of a periodic electrical field can be described by small oscillations of the polaron center of mass between the positions R_+ and R_- with occasional noise-driven abrupt transitions from R_- to R_+ and vice versa, across the unstable state R_0, which constitutes a potential barrier for such transitions:

$$\Delta U_\pm = U(R_0) - U(R_\pm). \tag{21}$$

The kinetics of these transitions depends on the potential barrier (21) and the noise strength $q^2 = 2\Gamma kT$.

In the limit of small temperatures, i.e., for small values of q^2 as compared to the local potential barrier $\Delta U_\pm$, the mean value of the transition between the two minima is given by the Kramers formula [37,38],

$$\tau_\pm^{-1} = \frac{M_s}{2\pi}\sqrt{\omega_0\omega_\pm}\exp\left(-\frac{\Delta U_\pm}{\Gamma kT}\right), \tag{22}$$

where

$$\omega_\pm = \frac{1}{M_s}\frac{d^2U}{dR^2}\bigg|_{R=R_\pm}, \quad \omega_0 = -\frac{1}{M_s}\frac{d^2U}{dR^2}\bigg|_{R=R_0}.$$

In the presence of the periodic electrical field $E(t)$ the corresponding barrier becomes a function of time: $V_\pm = \Delta U_\pm + E(t)$. As a result, there will be time moments when the states $R_\pm$ will be found at the bottom of the corresponding potential wells, which are successively less and more shallow than in the absence of the field. This can facilitate the system transitions between the two stable states, i.e., the temperature enhancement of the polaron drift. It has been known (see, e.g., [37]) that the equations of the type of Eq. (20) even for a symmetric quartic double-well ratchet potential lead to the stochastic resonance; this is even more true in the case of the asymmetric Peierls-Nabarro potential (17). And indeed, the numerical simulations of our discrete sets of equations demonstrate the existence of the stochastic resonance of a polaron drift in the oscillating electrical field subjected to thermal noise, as it is demonstrated in Fig. 4.

Before we conclude this paper, we would like to make a few general comments about our numerical results. One may wonder how much the results we have obtained are artifacts of our numerical procedures. In our simulations, the lattice always needed some time before is was fully thermalized and this thermalization took about 100 units of time. Most of our simulations were performed for 25 000 units of time and so the relaxation time was always small compared to the length of our simulations and had only a small impact on the measured drift. We are confident that the transient effects seen in Figs. 1 and 4 are not by-products of the lattice relaxation. On the other hand, when E is large, i.e., about $E > 0.2$, the polaron becomes unstable and decays after a few periods. In that case, the combined effect of the displacement and of the spreading of the polaron makes the evaluation of the drift difficult and unreliable.

V. CONCLUSIONS

In this paper we have studied the temperature dependence of the ratchet effect for large polarons in diatomic one-dimensional molecular chains. We had already shown in Ref. [6] that a polaron ratchet effect can be induced by a time periodic symmetric electric field in an asymmetric chain and in this paper we have studied the temperature dependence of this effect. As expected, the first effect of thermal noise is to introduce some randomness to the trajectory of the polaron. We have also observed that the thermal fluctuations facilitated the ratchet effect by lowering the critical value above which the polaron starts drifting. We have shown that there is a range of temperature values for which the drift at nonzero temperatures is stronger than at $T = 0$. For still higher temperatures thermal oscillations of the lattice sites become so strong that they compete with the polaron drift and decrease it. At high enough temperatures the polaron becomes unstable due to strong radiation of the linear waves and decays into a delocalized unbound state.

Temperature fluctuations lead to the lowering of the lower critical value of the field and this can be understood as follows: when the amplitude of the electric field is small, the polaron does not acquire enough energy to go over the energy barrier separating it from the next lattice site. With the thermal excitations present the polaron can get some extra energy from the thermal bath, which then helps it to overcome that energy

barrier and so leads to its drift at smaller values of the electric field. The thermal energy allows the polaron to move more easily between lattice sites and, as a consequence, the resulting effect is a somewhat larger displacement of the polaron within each period of the field and a stronger drift, up to a certain value of the electric field amplitude. In even stronger fields the polaron average drift decreases and at nonzero temperature becomes smaller than at $T = 0$.

Our results have a clear physical interpretation. At nonzero temperature the solution for the lattice displacements can be represented in the form of a sum of two terms $u = u_{n,j}^{(s\text{-}c)} + u_{n,j}^{(r)}$, where $u_{n,j}^{(s\text{-}c)}$ are self-consistent displacements due to the electron-lattice interaction, and $u_{n,j}^{(r)}$ are random displacements due to the nonzero temperature. This leads to the appearance of a random force in the dynamical equations for the polaron center-of-mass coordinate. On the other hand, the presence of random displacements $u_{n,j}(r)$ can also modify the polaron properties, because the Peierls-Nabarro potential now includes a random term as well. This extra term diminishes slightly the height of the lattice barrier and also "modifies" the asymmetry of the barrier. The effect depends on the amplitude of thermal vibrations, $A_{n,j} = \sqrt{\langle u_{n,j} u_{n,j} \rangle} \propto \sqrt{T}$. At sufficiently high temperatures this amplitude becomes comparable to the amplitude of self-consistent lattice displacements $u_{n,j}^{(s\text{-}c)}$. In consequence, the self-consistent lattice potential well becomes negligibly small and the polaron decays.

We have shown above that temperature has a significant effect on the dependence of the polaron drift on the period of the field. In particular, thermal vibrations of the lattice result in the decrease of the value of the lowest critical period of the field, at which the drift takes place. And we have also demonstrated that there is a stochastic resonance in the polaron ratchet phenomenon: there is an optimal temperature at which the polaron drift is largest. The values of the amplitude of the drift, of the stochastic resonance temperature, and of the critical values of the field intensity and its period depend on various parameters of the system and, in particular, on the anisotropy of the chain parameters. This temperature induced decrease of the critical value of the field intensity and its period, as well as the resonance itself, may be important for practical applications of the ratchet phenomenon in systems involving conducting polymers and other low-dimensional materials. It may also be important in some biological macromolecules where the ratchet phenomenon could take place in biomotors and energy and/or charge transport. Our results show that temperature effects on the dynamics of a polaron, in a lattice subjected to an unbiased external periodic force, are much more varied than in some other ratchet systems, such as kinks in an array of Josephson junctions. In the latter system the effect of the noise on the phenomenon is minimal, according to [39], in the sense that the dynamics of the kink gets dressed by the noise, but the average mean velocity of the kinks is almost the same as at zero temperature.

ACKNOWLEDGMENTS

One of us, L.S.B., acknowledges a Durham International Fellowship for Research and Enterprise (DIFeREns) COFUNDed by Durham University and the European Union for Ephiphany. She thanks St. Mary's College and the University of Durham for their hospitality. B.M.A.G.P. and W.J.Z. would like to acknowledge support from the STFC Grant No. ST/J000426/1.

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