Motion of a Classical Polaron in a dc Electric Field

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The motion of the classical polaron in a dc electric field is investigated numerically. In a limited range of parameters (field and coupling constant) a stable stationary asymptotic drift of the electron with a constant velocity is shown to exist. Outside this range of parameters the electron is asymptotically accelerated by the field, like a free charge. This model is an illustration of the dissipative behavior of a classical mechanical subsystem coupled to a mechanical system with an infinite number of degrees of freedom (here the classical LO phonon field).

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The model of an electron interacting with a longitudinal optical (LO) continuum phonon field through the Fröhlich coupling [1] is one of the basic quantum-mechanical models used in the description of polar solids. Many years ago Feynman [2] introduced a path integral formulation of this polaron model, in which the integration over the phonon variables is formally performed. The action functional of the polaron appearing under this path integral corresponds to a retarded self-interaction of the electron with itself. In spite of the many applications of the quantum-mechanical polaron model, its truly classical version got very little attention. About a decade ago some analytical asymptotic solutions with finite orbits [3-5] were found.

In this work the evolution of the system from an initial state at $t=0$ without polarization (no phonons) and an applied dc electric field collinear with the initial velocity of the particle is investigated. Therefore the solutions describe a one-dimensional collinear motion and do not include for vanishing dc field the finite orbit solutions of Refs. [3-5].

The main result of this paper is the analytical and numerical proof of the existence of stationary-flow asymptotic solutions in the presence of the dc electric field. This is an example of a dissipative asymptotic motion of a particle interacting with a system having infinitely many degrees of freedom (the phonon field). In recent years dissipative asymptotic results on a mathematically rigorous level have been obtained concerning the motion of a classical particle in a Rayleigh gas (see Ref. [6] for a comprehensive review). The peculiarity of the dissipative behavior described in this paper is that it is not of statistical nature, but refers to the trajectory of a single particle and describes a state with stationary flow.

Let us define briefly the model (although it may be found in many textbooks). It describes a polarization (dipole) density $\mathbf{P}(\mathbf{x})$, which in the absence of interaction $\mathbf{u}$ obeys an oscillator equation with the mass density μ and a single frequency ω_{LO}. This phonon field interacts with an electron of mass m and charge e through the Coulomb energy

$$-\frac{1}{\epsilon_\infty}\int d\mathbf{x}\int d\mathbf{y}\frac{\nabla\cdot\mathbf{P}(\mathbf{x},t)\rho(\mathbf{y},t)}{|\mathbf{x}-\mathbf{y}|},$$

where $\rho(\mathbf{x},t)=e\delta(\mathbf{x}-\mathbf{r}(t))$ is the charge density of the electron, $\mathbf{r}$ is the current coordinate of the electron, and ϵ_∞ is the background dielectric constant.

Unfortunately the model with Coulomb potential is mathematically ill defined due to the singularity at the origin. This is due to the idealization to an oscillator continuum contained in the above formulation. The phonons of solid-state physics are actually oscillations of a discrete lattice and the dangerous continuum idealization is usually repaired by restricting the wave vectors of the phonon (polarization) field to the first Brillouin zone, therefore assuring the conservation of the correct number of degrees of freedom (Debye trick). This is equivalent to the replacement of the Coulomb potential through a nonsingular cutoff potential $v(\mathbf{x};a)$ depending on a cutoff length a. The modification of the potential is such that

$$\lim_{a\to 0} v(\mathbf{x},a)=\frac{1}{|x|}\,.$$

Besides the interaction with the phonons we consider also an external dc electric field $\mathbf{E}$ acting on the electron.

The prototype of the classical polaron model we consider in the following is then described by the Lagrangian function

$$L=\frac{1}{2}\dot{\mathbf{r}}^2+\mathscr{E}\mathbf{r}+\int d\mathbf{x}\left\{\dot{\mathbf{u}}(\mathbf{x})^2-\mathbf{u}(\mathbf{x})^2+\left(\frac{C}{4\pi}\right)^{1/2}\nabla\cdot\mathbf{u}(\mathbf{x})v(\mathbf{x}-\mathbf{r})\right\},\quad(1)$$

where the inverse of the phonon frequency ω_{LO} was chosen as a unit of time, the cutoff length a as a unit of length, the energy unit is $m(\omega_{\mathrm{LO}}a)^2$, and the phonon field was rescaled to a dimensionless vector field $\mathbf{u}(\mathbf{x},t)$. After this rescaling it becomes obvious that the theory depends only on two dimensionless parameters, the coupling constant and the rescaled dc field,

$$C=\frac{e^2}{\epsilon^* m\omega_{\mathrm{LO}}^2a^3},\quad \frac{1}{\epsilon^*}\equiv\frac{4\pi e^2}{\mu\epsilon_\infty^2\omega_{\mathrm{LO}}^2},\quad \mathscr{E}=\frac{e}{ma\omega_{\mathrm{LO}}^2}E\,.$$

(For illustrational purposes, with a cutoff length $a=16$ Å and GaAs parameters $C\simeq 3.2$.)

Since only the longitudinal part of the phonon field is coupled to the electron, it is sufficient to concentrate on these longitudinal degrees of freedom. The coupled equations of motion follow as

$$\nabla\cdot\ddot{\mathbf{u}}(\mathbf{x},t)+\nabla\cdot\mathbf{u}(\mathbf{x},t)=-\left(\frac{C}{4\pi}\right)^{1/2}\nabla^2 v(\mathbf{x}-\mathbf{r}(t)),\quad(2)$$

$$\ddot{\mathbf{r}}(t)=\mathcal{E}-\left(\frac{C}{4\pi}\right)^{1/2}\int d\mathbf{x}\,\nabla v(\mathbf{x}-\mathbf{r}(t))\nabla\cdot\mathbf{u}(\mathbf{x},t).\quad(3)$$

One may eliminate the polarization charge in favor of the electronic variable through the formal solution of Eq. (3). We shall do this by choosing a special solution of the inhomogeneous equation adequate for defining an initial value problem at $t=0$. We chose a vanishing polarization in the absence of the electron charge (introduced at $t=0$); then

$$\nabla\cdot\mathbf{u}(\mathbf{x},t)=-\left(\frac{C}{4\pi}\right)^{1/2}\int_0^t dt'\sin(t-t')\nabla^2 v(\mathbf{x}-\mathbf{r}(t')).\quad(4)$$

This polarization charge density induced by the electron is nonvanishing only along the path of the electron within a tube whose transverse dimension is given by the cutoff length. Introducing this result into the Newton equation of the electron one gets the closed equation for the electron (from now on to be called polaron)

$$\ddot{\mathbf{r}}(t)=\mathcal{E}+C\int_0^t dt'\sin(t-t')\frac{\partial}{\partial\mathbf{r}(t)}V(\mathbf{r}(t)-\mathbf{r}'(t)),\quad(5)$$

where a new potential V was introduced according to the definition

$$V(\mathbf{r})\equiv-\frac{1}{4\pi}\int d\mathbf{x}\,v(\mathbf{r}-\mathbf{x})\nabla^2 v(\mathbf{x}).\quad(6)$$

If one chooses for $v(\mathbf{x})$ to be the Coulomb potential, one gets for $V(\mathbf{r})$ again the Coulomb potential, but otherwise the two are different. Nevertheless, if one chooses a cutoff procedure in which the "smoothed point charge" $\rho(\mathbf{x})\equiv-\frac{1}{4}\pi\nabla^2 v(\mathbf{x})$ falls off sufficiently rapidly away from $\mathbf{x}=0$, the potential $V(\mathbf{r})$ will be also Coulomb-like.

One sees that it is convenient to consider the potential $V(\mathbf{r})$ as the primary quantity instead of $v(\mathbf{r})$. We chose for our calculations a simple analytical form for this potential which is regular in the origin, and Coulomb-like at large distances

$$V(\mathbf{r})\equiv(r^2+1)^{-1/2}.\quad(7)$$

In what follows we shall consider only collinear motions, which are the only solutions if the initial velocity of the electron is collinear with the field, and arrive at the one-dimensional equation

$$\frac{d^2x(t)}{dt^2}=-C\int_0^t dt'\sin(t-t')\frac{x(t)-x(t')}{\{[x(t)-x(t')]^2+1\}^{3/2}}+\mathcal{E}.\quad(8)$$

The solution is completely determined by giving the coordinate and the velocity of the polaron at $t=0$.

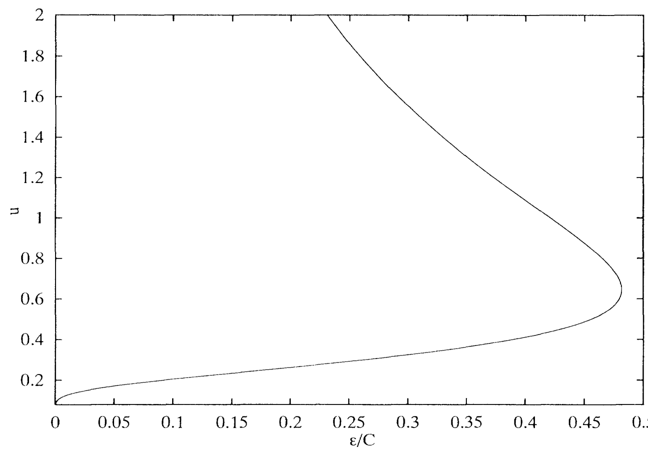

FIG. 1. Possible (asymptotical) stationary-flow velocities of the polaron u as a function of the ratio of the field $\mathcal{E}$ to the coupling constant C.

Equation (11) is a nonlinear integrodifferential equation with infinite memory and therefore finding its general solution analytically is hopeless.

Let us assume that there is a solution in the presence of the field, which "very rapidly" develops into a stationary motion with constant velocity v:

$$x(t)\to ut.$$

A necessary condition for this velocity is

$$0=-C\int_0^\infty dt\sin t\frac{ut}{[(ut)^2+1]^{3/2}}+\mathcal{E},\quad(9)$$

which leads to the transcendental equation (in terms of a Bessel function)

$$\mathcal{E}=\frac{C}{u^2}K_0\left(\frac{1}{u}\right).\quad(10)$$

The dependence of the asymptotically stationary velocity u on $\mathcal{E}/C$ is represented in Fig. 1. It is clear that above a certain field ($\mathcal{E}_{max}\simeq0.483C$), which is the upper bound of the momentum transfer rate to the phonons in a uniform motion, no asymptotically stationary-flow solutions are possible. It is worth mentioning that in order to sustain a stationary flow with a finite (unscaled) velocity au as $a\to0$, according to Eq. (8) one needs an infinite (unscaled) field E.

Of course the existence of such an asymptotically stationary solution is not yet shown, but just a necessary criterion for its existence was found. Unfortunately a standard stability analysis is not possible. First of all, we do not know the exact solution but just its asymptotically leading term. Second, any linearized version of the theory, due to the memory effects looks even more complicated than the original nonlinear equation.

The very existence and stability (against variations of the initial velocity) of the stationary drift solutions will be shown only numerically. Equation (8) has indeed a very

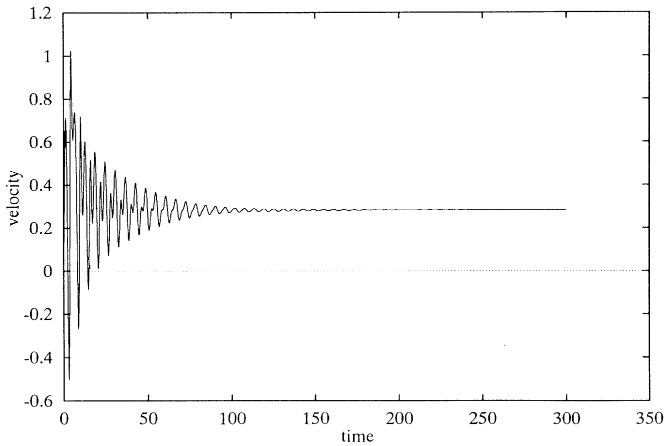

FIG. 2. Velocity of the polaron as a function of time in the presence of a field $\mathcal{E}=0.75$ at a coupling constant $C=3.2$. The initial velocity was taken to be zero.

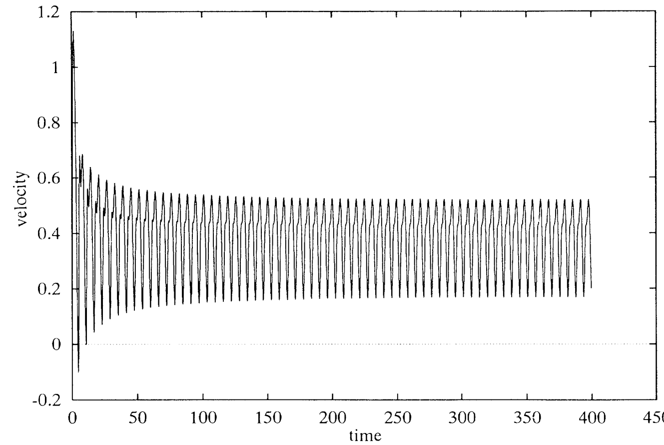

FIG. 4. Velocity of the polaron as a function of time in the presence of a field $\mathcal{E}=1.25$ at a coupling constant $C=3.2$. The initial velocity was taken to be -2.0.

simple structure, which is easy to translate into a rapidly converging discrete numerical algorithm. In what follows, numerical solutions of this equation obtained on a work station are reported.

All the solutions found for various coupling constants, fields, and initial velocities may be classified in one of two categories: (a) paths which asymptotically tend to a uniform drift, whose velocity (within some error) lies on the lower branch of the curve of Fig. 1; and (b) paths which asymptotically tend to the uniformly accelerated motion of the noninteracting electron in the external dc field.

The example given in Fig. 2 illustrates a trajectory of the first category. At a coupling constant $C=3.2$ in the presence of a field $\mathcal{E}=0.75$, after starting with an initial velocity $\dot{x}(0)=0$, one very rapidly obtains a steady motion, whose velocity corresponds to the asymptotically predicted value. Under the same parameters, but an initial velocity $\dot{x}(0)=1.5$, the trajectory suddenly changes its nature and becomes uniformly accelerated as is shown in Fig. 3. The same kind of transition to accelerated motion occurs if the initial velocity $\dot{x}(0)=0$ of the electrical field is increased to $\mathcal{E}=1.25$, although this is still smaller than the maximally allowed momentum transfer rate given for this coupling constant by $\mathcal{E}_{\max}\simeq 1.5456$. Nevertheless, an asymptotic motion with a constant drift may be again realized if the initial velocity is taken opposite to the direction of the field $\dot{x}(0)=-2.0$. Above the maximal field of 1.5456 the asymptotical motion is always uniformly accelerated.

It can be easily seen from Eq. (4) that in the asymptotically steady drift motion the induced polarization charge density closely follows the electron, and it is well approximated by a running wave with the phase velocity v and the phonon frequency along the electronic path. At the same time it can be shown that the energy of the phonon system increases linearly with the time, while the interac-

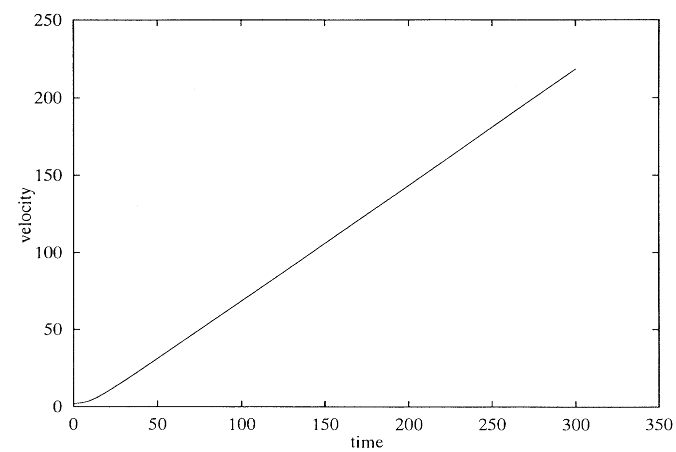

FIG. 3. Velocity of the polaron as a function of time in the presence of a field $\mathcal{E}=0.75$ at a coupling constant $C=3.2$. The initial velocity was taken to be 1.5.

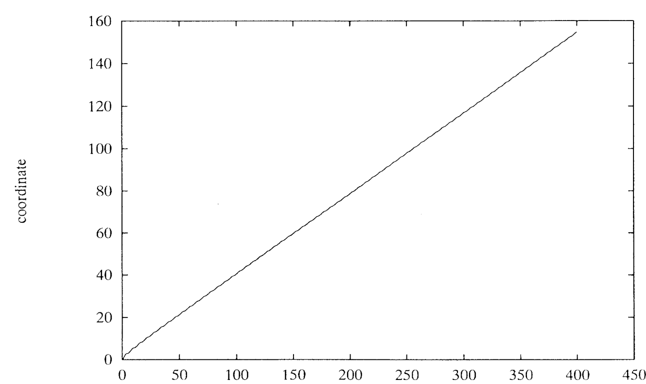

FIG. 5. Coordinate of the polaron as a function of time in the presence of a field $\mathcal{E}=1.25$ at a coupling constant $C=3.2$. The initial velocity was taken to be -2.0.

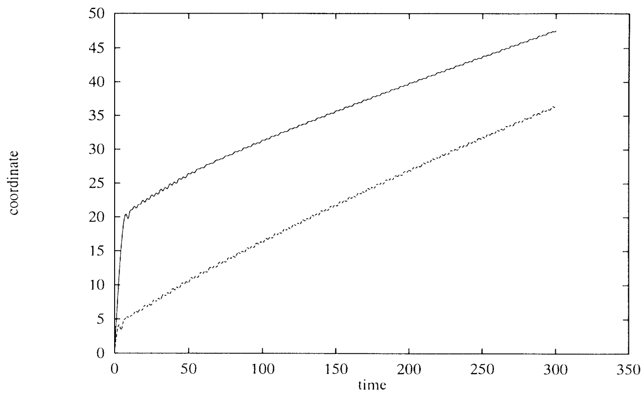

FIG. 6. Coordinate of the polaron as a function of time in the absence of a field for a coupling constant $C=3.2$. The initial velocity for the two trajectories was taken to be 2.0 and 4.0, respectively.

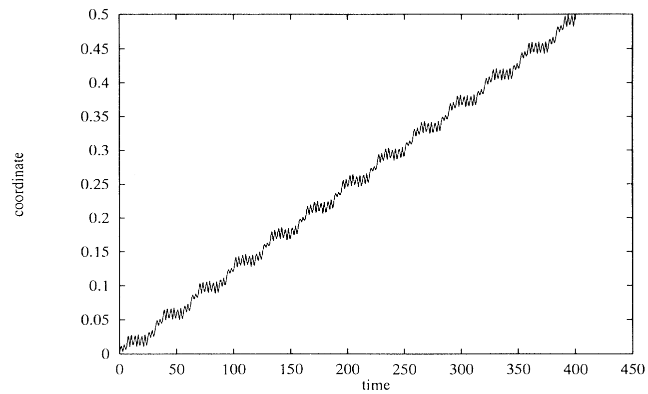

FIG. 7. Coordinate of the polaron as a function of time in the absence of a field at a coupling constant $C=3.2$, for an initial velocity of 0.01.

tion energy remains asymptotically constant. If during the initial stage of the motion, which is mainly determined by the initial velocity of the electron and the applied field (ballistic motion), the electron does not lose its contact to the polarization charge, then steady motion follows asymptotically, if in the same time the field strength does not exceed the maximal momentum transfer rate $\mathcal{E}_{\max}$.

On the contrary, in the asymptotically accelerated motion the polarization charge density decreases as $1/t$ at any finite distance behind the electron. The electron loses its polarization cloud and the interaction energy vanishes as $1/t$. This kind of asymptotic behavior follows whenever, either due to the high initial velocity or high field already in the initial (ballistic) state of the motion, the electron leaves its polarization charge far behind.

On the grounds of the discussion above it is also understandable why no drift solutions on the upper branch of the stationary curve, having high velocities, were found.

A closer inspection (blowup) of Fig. 2 actually shows small amplitude oscillations, which decay very slowly, if at all. These oscillations are well pronounced in the case of the drift motion at $C=3.2$ and $\mathcal{E}=1.25$ and $\dot{x}(0)=-2.0$ shown in Fig. 4. Nevertheless, the path of this polaron in Fig. 5 shows a clear constant average drift velocity of 0.455, slightly above the expected ideal value of 0.41. The ground frequency of the oscillations is always 1 (the phonon frequency); however, it has many higher harmonics. The deviation of the drift velocity from its ideal value might be attributed either to the fact that the true asymptotic regime was not yet achieved, or rather to the rough asymptotical analysis, which took only the leading asymptotic term into account.

The above described scenario has been checked by various coupling constant strengths, fields, and initial velocities.

Strong asymptotic oscillations are also typical for very low fields. Therefore, although in the absence of the electric field according to Fig. 1 the asymptotical drift velocity should vanish, we cannot exclude oscillating slow asymptotic drift solutions. According to the numerical experience, the motion of the electron in the absence of a dc field first suffers a rapid slowdown and afterward a very slow drift regime sets in. In Fig. 6, two trajectories are represented for $C=3.2$ having two different initial velocities [$\dot{x}(0)=2.0$ and 4.0]. The drift velocity of the slow motion is, however, not constant. One of the trajectories was followed over a long time duration ($t=1000$) and we found that the average drift coordinate increases sublinearly approximately as $t^{0.85}$. We cannot decide, however, on the basis of our numerical results, whether the motion is asymptotically very slowly damped, or a steady asymptotic drift regime with a very small velocity will be achieved. It is also relevant that for very small initial velocities the oscillatory component of the motion has a very complicated structure like that shown in Fig. 7 for $\dot{x}(0)=0.01$ and $C=3.2$ and no damping could be put into evidence.

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