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Properties of the moving Holstein large polaron in one-dimensional molecular crystals

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Abstract
The features of the moving large polaron are investigated within Holstein's molecular crystal model. The necessity to account for the phonon dispersion is emphasized and its impact on polaron properties is examined in detail. It was found that the large polaron dynamics is described by the nonlocal nonlinear Schrödinger equation. The character of its solutions is determined by the degree of nonlocality, which is specified by the polaron velocity and group velocity of the lattice modes. An analytic solution for the polaron wavefunction is obtained in the weakly nonlocal limit. It was found that the polaron velocity and phonon dispersion have a significant impact on the parameters and dynamics of large polarons. The polaron amplitude and effective mass increase while its spatial extent decreases with a rise in the degree of nonlocality. The criterion for the stability of large polaron is formulated in terms of the values of the degree of nonlocality, the magnitude of the basic energy parameters of the system and the polaron velocity. It turns out that the large polaron velocity cannot exceed a relatively small limiting value. A similar limitation on large polaron velocity has not been found in previous studies. The consequences of these results on polaron dynamics in realistic conditions are discussed.

1. Introduction

It has been argued for a long time that the large polaron may have a substantial role in the long distance charge and energy transfer in quasi-one-dimensional conductors and some biological macromolecules, such as the α-helix and DNA [1–11]. These ideas were founded upon quite general theoretical arguments [2, 12–14] which indicate that an excess electron (hole, exciton, etc.) in a one-dimensional electron–phonon system will always self-trap to form a one-dimensional polaron, irrespective of the strength of the electron–phonon interaction. The polaron spatial extent varies with the values of system parameters and compact, soliton-like, large polaron states extending over a few lattice sites appear in the adiabatic limit (electron bandwidth greatly exceeds maximal phonon energy) provided that the intersite transfer energy exceeds the electron–phonon coupling energy. This polaron is extremely stable to external perturbations and may propagate through the crystal as a robust, massive classical particle carrying the charge and energy over large distances. For all these reasons it was speculated that the transport processes in various quasi-1D substances may be achieved by a polaronic mechanism. Such a belief was supported by many examples of experimental evidence of polaron formation in a broad class of materials, such as quasi-1D conductors (MX-chains, conducting polymers, etc.) [9, 15, 16].

On the theoretical side, the polaron problem has been exhaustively investigated and we now have a comprehensive description of polaron features over practically the whole parameter space [1–14, 17–25]. Nevertheless, despite all

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these efforts, some details are still only poorly understood. One of these problems concerns the large polaron motion in quasi-one-dimensional molecular crystals, which has mainly been studied within idealized 1D models. However, external forces, disorder, three-dimensional effects, etc., are inevitable in realistic conditions and should be taken into account in the investigation of the possible role of polarons in transport processes in these substances. One of the effects which was not so far been satisfactory treated in polaron theory concerns taking into account the influence of the phonon dispersion on polaron properties. Namely, theoretical investigations of polarons in 1D systems were mainly carried out within the dispersionless (phonon dispersion is neglected) Holstein's molecular crystal model [2]. Such a practice greatly simplifies particular calculations, but it is not generally acceptable and may lead to erroneous results. In particular, some studies of small polaron properties, in various contexts, have clearly shown the necessity of accounting for phonon dispersion. Thus for example, Zoli, Zoli and Das [19] found that ignoring the phonon dispersion, even accounting for it within the common weak dispersion approximation, would lead to the overestimation of the polaron bandwidth and divergent site jump probabilities in one-dimensional systems. Moreover, De Raedt and Lagendijk [20] examined, numerically, the impact of phonon dispersion on transition between free and self-trapped electron states. They found significant correlations between the gap in the optical phonon spectrum and the value of the critical coupling constant below which the self-trapping (ST) transition does not occur.

Dispersion of optical phonons has, until recently, been mostly ignored in the studies of the large polaron motion. Some recent investigations [17] imply that phonon dispersion may be important for the proper description of the moving Fröhlich polaron. On the other hand, to our best knowledge, these effects have never been accounted for in studies of the moving large polaron properties within Holstein's molecular crystal model. The aforementioned references [19, 20] do not represent an exception in that sense, since they strictly focus on other important issues such as the impact of phonon dispersion on the polaron transition from the free to the ST state. In the present paper we shall examine this hitherto ignored problem: the impact of phonon dispersion on the properties of the moving large polaron. Our research is motivated by the assumed, possibly significant, role of the polaron mechanism in charge and energy transfer in quasi-1D molecular structures. Further analysis will be carried out within the adiabatic limit in which formation of the large polaron is expected. We hope that our efforts will shed some light on these problems.

In section 2 we review the main results of the traditional adiabatic strong coupling theories, pointing out the limits of their applicability. In section 3 the nonlocal nonlinear Schrödinger equation for polaron wavefunction is derived. Special attention is payed to the clarification of the continuum approximation. In section 4 the explicit form of polaron wavefunction is found in the weak nonlocal limit. Polaron properties, in particular stability, are discussed on the basis of that result. Section 5 contains the calculation of the polaron effective mass and energy; finally, a brief survey of our results is given in section 6.

2. Adiabatic large polaron preliminaries

The starting point of our analysis is the one-dimensional Hamiltonian of Holstein's molecular crystal model [2]

$$H = -J \sum_{n,l=\pm 1} A_n^\dagger A_{n+l} + \sum_q \hbar\omega_q b_q^\dagger b_q + \frac{1}{\sqrt{N}} \sum_{q,n} F_q \mathrm{e}^{\mathrm{i}qnR_0} A_n^\dagger A_n (b_q + b_{-q}^\dagger). \tag{1}$$

Here n labels lattice sites and R_0 denotes the lattice constant along the chain. Easy transfer along the chain is associated with nearest neighbor transfer integral J; operator $A_n^\dagger(A_n)$ describes the presence (absence) of the electron on the nth lattice site; $b_q^\dagger(b_q)$ creates (annihilates) a phonon quanta with the frequency ω_q; $F_q = \chi\sqrt{\frac{\hbar}{2M\omega_q}}$ denotes the electron–phonon coupling parameter where χ represents the strength of this interaction. Finally, $\omega_q = \sqrt{\omega_0^2 + \omega_1^2 \cos q R_0}$ denotes the phonon frequency, where ω_0 denotes the frequency of the intramolecular oscillations, while ω_1 characterizes the vibrational energy transfer between neighboring sites. We may assume that polaron spatial extent highly exceeds the lattice constant. This justifies the continuum approximation, and for the practical calculation we will use an approximate expression $\omega_q \approx \sqrt{\Omega_0^2 - c^2 q^2}$. Here $\Omega_0 = \sqrt{\omega_0^2 + \omega_1^2}$ while $c = \sqrt{\frac{R_0^2\omega_1^2}{2}}$.

Polaron properties as well as the choice of the method for its theoretical description are determined by the mutual ratio of: $2J$, the electron bandwidth, $\hbar\Omega_0$, the maximal phonon energy, and the small polaron binding energy $E_{\mathrm{B}} = \frac{1}{N}\sum_q \frac{|F_q|^2}{\hbar\omega_q}$ [13]. The last parameter denotes the energy gained by the polaron formation in the transportless limit ($J = 0$) when the carrier is confined to a single site. It is sometimes termed the lattice relaxation energy, electron–phonon coupling energy or lattice deformation energy [13]. In particular, most aspects of polaron physics may be characterized in terms of just two parameters: the adiabatic ratio $B \sim \frac{2J}{\hbar\Omega_0}$ and the coupling constant,$S \sim \frac{E_{\mathrm{B}}}{\hbar\Omega_0}$. Sometimes, another coupling parameter, $\lambda \sim \frac{E_{\mathrm{B}}}{J}$, directly related to polaron size in units of lattice constant ($L_{\mathrm{p}}/R_0 \sim 2J/E_{\mathrm{B}}$), is used.

Large adiabatic polarons may be successfully described using Pekar's variational method [12]. It relies upon the semiclassical treatment of a phonon subsystem which is considered to be very slow as compared to the electronic one. Accordingly, the polaron wavefunction may be decomposed into the product of the electron and lattice part. The large polaron motion has usually been studied by means of the stationary Pekar's method supplemented by the requirement that the total momentum of the electron–lattice system is the integral of the motion. In such an approach the polaron velocity is introduced as a Lagrange multiplier [5]. An alternate possibility represents the time dependent variant of this method, now widely known as Davydov's ansatz [3, 4, 22, 26]. It has some practical advantages and will be used here.

The unfounded application of the time dependent ansatz, beyond the limits of the applicability of semiclassical approximation, had raised some doubts as to its validity [26–28].

This criticism is only partially justified, since, within the limits of the applicability of the stationary theory of Pekar *et al* [1, 2, 5, 8, 12], time dependent theory provides a reliable basis for the description of large polaron properties. Nevertheless, in order to avoid any possible confusion or doubts about the reliability of our further results, we now briefly review the conditions which ensure the applicability of the semiclassical variational approach. For a detailed discussion on that subject we refer the reader to literature on the classical polaron [1, 2, 5, 12]. At this stage we emphasize only the main points: the validity of the semiclassical variational method of Pekar [12] and its nonstationary counterpart [3, 4, 22] demands the fulfilment of the adiabatic ($2J \gg \hbar\Omega_0$) and strong coupling conditions ($S \gg 1$). The first of these conditions provides the applicability of the semiclassical factorization of the wavefunction, while the second one ensures polaron stability in respect to the linear modes. The latter condition originates from the demand that phonons cannot excite an electron from the potential well in which it is trapped. This means, quantitatively, that the polaron binding energy exceeds the maximal phonon energy $E_{\mathrm{B}} \gg \hbar\Omega_0$ [8] and coincides with the strong coupling condition ($S \gg 1$). In addition, the applicability of the continuum approximation demands that the polaron radius must exceed the lattice constant ($L_{\mathrm{p}}/R_0 > 1 \Leftrightarrow 2J > E_{\mathrm{B}}$). This imposes an upper bound on the value of the coupling constant which cannot be arbitrarily large and must satisfy $S < B$. If $S > B$ the polaron radius is restricted to the lattice constant and formation of the adiabatic small polaron takes place. A detailed study of the small to large polaron transition in the adiabatic limit is presented in [23] within the dispersionless Holstein model.

Results of the recent numerical simulations [24] and Monte Carlo simulations [25] confirm the validity of the adiabatic variational method under the aforementioned conditions. Hereafter, our analysis concerns the problem of the moving large polaron and, therefore, we assume that system parameters satisfy $B \gg 1$, $S \gg 1$ and $S < B$.

Concerning the relevance of our analysis to the understanding of polaron properties in realistic conditions, we emphasize that the aforementioned criteria could be satisfied in a wide class of realistic substances. In particular, the adiabatic criterion is satisfied in conducting polymers such as polyacetylene and related materials [9], in which the electron next neighbor overlap integral is in the range of a few electron volts ~2.5–5.6 eV; the characteristic phonon frequencies are estimated to be of the order of 0.12 eV. On the other hand, there is some controversy over the estimates of the value of J in biological materials [11] so that fulfilling the adiabatic condition in these materials is questionable. In particular, the actual estimates of J in DNA sometimes differ up to an order of magnitude; roughly ranging from 0.02 eV [10] up to 0.2 eV [11]. Phonon frequencies are typically about few 100 meV. The usually quoted value of the electron–phonon coupling parameter in conducting polymers is 4.1 eV Å^{-1} [9] while, again, in biological macromolecules a certain controversy exists as to the actual value of this parameter. Some estimates implies that its value is about ten times less than that of conducting polymers: 0.6 eV Å^{-1} [11]. Direct calculations confirm the belief that the criteria are fulfilled for large polaron existence in conducting polymers, while its formation in aforementioned biological macromolecules is still open to question.

In the existing literature there are no reliable data on the value of ω_1 for any realistic substances. However, beginning with the pioneering article by Holstein [2], it was usually regarded to be very small in comparison with ω_0. This assumption does not hold in the general case. In particular, in recent studies of the small polaron properties [19], it was found that ω_1 cannot be arbitrarily small. That is, it should not exceed some minimal value determined by the system dimensionality, magnitude of coupling constant and ω_0. In one-dimensional systems this threshold value approaches $(2/3)\omega_0$ in the strong coupling limit. However, the aforementioned restrictions on the values of ω_1 strictly concern the small polaron limit in which the quantum nature of the phonon field dominates and should not be relevant for the present purposes. Thus we may ignore the lower boundary for ω_1 and we assume that it ranges from zero up to a few tenth of ω_0, for which we adopt the typical value for one-dimensional conductors: $\omega_0 \sim 0.12$ eV. In such a way we may take it that Ω_0 ranges up to $1.5\omega_0$, which cannot substantially affect the adiabatic condition due to large values of the hopping term J.

Under the above conditions we may safely proceed as proposed and we choose [3] the time dependent trial state as follows

$$|\Psi(t)\rangle = \sum_n \Psi_n(t) A_n^{\dagger}|0\rangle_e \otimes |\beta(t)\rangle, \qquad \sum_n |\Psi_n|^2 = 1. \tag{2}$$

Here Ψ_n denotes the electron wavefunction while the phonon part is the functional of phonon coherent amplitudes. In particular, $|\beta(t)\rangle$ is a multimode coherent state defined as the total product of single mode phonon coherent states $|\beta(t)\rangle = \prod_q |\beta_q(t)\rangle \equiv \exp\{\sum_q(\beta_q(t)b_q^{\dagger} - \beta_q^*(t)b_q)\}|0\rangle_{\mathrm{ph}}$.

Functions Ψ_n and β_q will be treated as dynamical variables and the evaluation of their evolution in time is now our primary task. For that purpose we utilize the time dependent variational principle from which we derive the evolution equations demanding the stationarity of the action functional $A = \int_{t_1}^{t_2} \mathcal{L}(\Psi, \Psi^*; \beta_q; \beta_t^*)\,\mathrm{d}t$, where $\mathcal{L}(\Psi, \Psi^*; \beta_q; \beta_t^*) = \frac{\mathrm{i}\hbar}{2}(\langle\Psi|\dot{\Psi}\rangle - \langle\dot{\Psi}|\Psi\rangle) - \langle\Psi|H|\Psi\rangle$ denotes system Lagrangian. Thus, imposing $\delta A = 0$, we obtain the following set of Hamilton's equations:

$$\mathrm{i}\hbar\dot{\Psi}_n = \frac{\delta\mathcal{H}}{\delta\Psi_n^*}; \qquad \mathrm{i}\hbar\dot{\beta}_q = \frac{\delta\mathcal{H}}{\delta\beta_q^*}. \tag{3}$$

Here $\mathcal{H} \equiv \langle\Psi|H|\Psi\rangle$ denotes the classical Hamiltonian (Hamilton's function).

The equation of motion for β_q reads

$$\mathrm{i}\hbar\dot{\beta}_q = \hbar\omega_q\beta_q + \frac{1}{\sqrt{N}}\sum_n F_{-q}\mathrm{e}^{-\mathrm{i}q\cdot nR_0}|\Psi_n(t)|^2. \tag{4}$$

This equation is readily solved after passing to a continuum approximation and assuming that the polaron probability density $|\Psi(x,t)|^2$ depends on time only through the coordinate in the moving frame, i.e. $|\Psi(x,t)|^2 = |\Psi(x - vt)|^2$, where

v represents the polaron velocity. Then, by virtue of the substitution $y = x - vt$, equation (4) becomes an ordinary inhomogeneous differential equation of the first order. Only the stationary case, (v = const), will be considered hereafter. This yields

$$\beta_q(t) = \beta_q(0)\mathrm{e}^{-\mathrm{i}\omega_q t} - \frac{1}{\sqrt{N}} \frac{F_{-q}\mathrm{e}^{-\mathrm{i}qvt}}{\hbar(\omega_q - qv)} \int \frac{\mathrm{d}x}{R_0}\mathrm{e}^{-\mathrm{i}qx}|\Psi(x)|^2. \tag{5}$$

The first term corresponds to a homogeneous solution of equation (4) and describes the influence of the phonon fluctuations on the large polaron dynamics. It is irrelevant in the present context and will be disregarded hereafter in accordance with the common approximations used in adiabatic large polaron theories. That is, in what follows we shall keep only the particular solution of equation (4), corresponding to the so called frozen (coherent) part of lattice distortion coherently following the electron motion.

3. Nonlocal nonlinear Schrödinger equation

Substituting the particular solution for lattice amplitudes (5) into the equation of motion for the polaron wavefunction we obtain the nonlocal nonlinear Schrödinger equation (NLNSE)

$$\mathrm{i}\hbar\dot{\Psi}(x,t) + JR_0^2\Psi_{xx}(x,t) + 2E_\mathrm{B}^0 \int \frac{\mathrm{d}x'}{R_0}\mathcal{K}(x-x')|\Psi(x',t)|^2\Psi(x,t) = 0, \tag{6}$$

where $E_\mathrm{B}^0 = \frac{\chi^2}{2M\Omega_0^2}$ is the small polaron binding energy in the continuum approximation for phonon modes, while $\mathcal{K}(x)$ denotes the following Green function

$$\mathcal{K}(x) = \frac{1}{N}\sum_q \frac{\mathrm{e}^{\mathrm{i}qx}}{1-\zeta^2q^2} \approx \frac{R_0}{2\pi}\int_{-\pi/R_0}^{\pi/R_0} \frac{\mathrm{d}q\,\mathrm{e}^{\mathrm{i}qx}}{1-\zeta^2q^2}. \tag{7}$$

It accounts for the nonlocality of the electron–phonon interaction, whose range is determined by the magnitude of the correlation length: $\zeta = \frac{R_0\omega_1}{\sqrt{2}\omega_0}\sqrt{\frac{1+(v/c)^2}{1+(\omega_1/\omega_0)^2}}$.

Equations of the above type arise in the theoretical description of various phenomena including: many-body quantum systems treated in Hartree approximation, optics, plasmas, Bose–Einstein condensation, etc. [29–33]. The character of the solutions of the above equation is determined by the magnitude of the ratio of the interaction range, ζ, and the characteristic scale of the spatial variation of the wavefunction (the polaron radius in the present case). One may get an intuitive insight into how this ratio affects the solutions of the NLNSE (6) by means of a scale change of the polaron wavefunction [33] $\Psi(x) \to \frac{1}{\sqrt{l_\mathrm{p}}}\Psi(\frac{x}{l_\mathrm{p}})$, where parameter $l_\mathrm{p} = L_\mathrm{p}/R_0$ has the meaning of the polaron radius in units of the lattice constant. After some simple manipulation, including variable changes $x \to x/l_\mathrm{p}$ and $q \to ql_\mathrm{p}$, followed by the replacement of the integration boundary in equation (7) $\pi/R_0 \to \pi/(R_0/l_\mathrm{p})$, this procedure results in a mathematically identical evolution equation but with scaled coefficients and correlation length $\zeta(L_\mathrm{p}) = \zeta/L_\mathrm{p}$. In the present case this ratio may be regarded to be very small. This is ensured by the assumed smallness of the ratio ω_1/ω_0 and the fact that the large polaron, by definition, is spread over a large number of lattice sites. Under these circumstances the soliton (polaron) spatial extent highly exceeds the characteristic extent of nonlocality, so that $\zeta/L_\mathrm{p} \ll 1$ provided that the polaron velocity is not too large. This case is known in the literature as the weakly nonlocal limit. It may successfully be treated approximately by expanding the kernel (7) in terms of the small parameter ξ^2 ($\xi = \zeta/R_0$, the nonlocality parameter). Note, however, that the increasing of the polaron velocity towards the minimum optic phonon phase velocity, $c_\mathrm{p} = \Omega_0R_0/\pi$, may violate the validity of such an approximation. Therefore, our analysis hereafter concerns the limit $v \ll \Omega_0R_0/\pi$, so that we may safely approximate kernel (7) as follows:

$$\mathcal{K}(x) \approx \left(1 - \xi^2\frac{\partial^2}{\partial x^2}\right)\delta(x). \tag{8}$$

Consequently, equation (6) becomes

$$\mathrm{i}\Phi_\tau(x,\tau) + \Phi_{xx}(x,\tau) + |\Phi(x,\tau)|^2\Phi(x,\tau) - \xi^2\frac{\partial^2|\Phi(x,\tau)|^2}{\partial x^2}\Phi(x,\tau) = 0. \tag{9}$$

Here the integration limit in equation (7) is extended towards infinity, which is justified if the polaron size greatly exceeds the lattice constant.

For practical reasons the last two equations were written in a dimensionless form introducing the new 'time' ($\tau = tJ/\hbar$) and 'spatial' $x' = x/R_0$ variables, while $\Phi = \sqrt{\frac{2E_\mathrm{B}^0}{J}}\Psi$ denotes the renormalized polaron wavefunction. Primes will be neglected hereafter, i.e. $x' \to x$. It is obvious that the nonlinear dynamical behavior of this system, as well as its stationary states, crucially depend on the interplay of the local and derivative nonlinear terms.

4. Polaron solution in the weak nonlocal limit

We search for the solutions of the above equation in the form $\Phi(x,\tau) = \mathrm{e}^{\mathrm{i}kx+\mathrm{i}(\Gamma-k^2)\tau}\phi(u)$, where the polaron envelope ϕ is a real, symmetric and exponentially localized ($\phi(0) = \phi_0, \phi(\pm\infty) = 0$) function of the polaron coordinate in the moving frame $u = x - \nu\tau$ ($\nu = v\frac{\hbar}{JR_0}$, the polaron velocity in dimensionless units). Separating the imaginary and real parts in equation (10) we found $k = \nu/2$, while the equation for the polaron profile reduces to

$$\phi_{uu} - \Gamma\phi + \phi^3 - \xi^2\left(\phi^2\right)_{uu}\phi = 0. \tag{10}$$

Its first integral is

$$\phi_u^2(1 - 2\xi^2\phi^2) + \tfrac{1}{2}\phi^2(\phi^2 - 2\Gamma) = C. \tag{11}$$

Imposing the polaron initial conditions $\phi(0) = \phi_0$ and $\phi_u(0) = 0$ we found the relation connecting the soliton amplitude and frequency, $\phi_0^2 = 2\Gamma$. On the other hand, the boundary conditions $\phi(\pm\infty) = 0$ and $\phi_u(\pm\infty) = 0$ yield $C = 0$, so that the equation for the polaron profile reduces to

$$\phi_u^2 = \frac{1}{2}\frac{\phi^2(\phi_0^2 - \phi^2)}{1 - 2\xi^2\phi^2}. \tag{12}$$

Final integration may be achieved by virtue of the substitution $\phi = \phi_0 \cosh \varphi(u)$, which yields the exact solution for the polaron profile in the implicit form

$$\pm u = -\frac{1}{\sqrt{2}\phi_0} \ln \left| \frac{\phi_0\sqrt{1-2\xi^2\phi^2} + \sqrt{\phi_0^2-\phi^2}}{\phi_0\sqrt{1-2\xi^2\phi^2} - \sqrt{\phi_0^2-\phi^2}} \right| + 2\xi \ln \frac{2\xi\sqrt{\phi_0^2-\phi^2} + \sqrt{1-2\xi^2\phi^2}}{\sqrt{1-2\xi^2\phi_0^2}}. \tag{13}$$

In the local limit ($\xi = 0$) only the first term survives and the above solution attains a typical bell-shaped soliton form. In the case of a nonvanishing nonlocality the two components of this solution compete with each other causing deformation of the soliton profile: an increase of the polaron amplitude followed by a reduction of its spatial extent. The degree of these modifications is determined by the polaron amplitude, which must be evaluated in terms of system parameters. For that purpose we exploit the normalization condition $\int_{-\infty}^{\infty} \mathrm{d}x/R_0|\Psi|^2 = 1 \Leftrightarrow \int_{-\infty}^{\infty} \mathrm{d}x\,|\Phi|^2 = 2E_\mathrm{B}^0/J$. This integral may be easily evaluated by employing the identity $\int |\Phi|^2\,\mathrm{d}x = \int \phi^2\,\mathrm{d}u \equiv \int \phi^2/\phi_u\,\mathrm{d}\phi$, which finally yields the implicit equation for the polaron amplitude

$$\mathcal{N} = \Phi_0 + \frac{(1-\Phi_0^2)}{2} \ln\left|\frac{1+\Phi_0}{1-\Phi_0}\right|. \tag{14}$$

For convenience, the scaled variables: norm $\mathcal{N} = \frac{2E_\mathrm{B}^0\xi}{J}$, profile function $\Phi = \sqrt{2}\xi\phi$ and amplitude $\Phi_0 = \sqrt{2}\xi\phi_0$ were introduced.

One cannot find the exact solution of equation (14) for polaron amplitude Φ_0 for an arbitrary value of the rescaled norm. However, instead, one may plot norm $\mathcal{N}$ as a function of Φ_0, which may be easily inverted to give the desired dependence of the polaron amplitude on the system parameters. Results are presented in figure 1. Note that, by virtue of the equation (13), which imposes $2\xi^2\phi_0^2 < 1$, all physically meaningful solutions of the last equation lie in the interval $0 < \Phi_0 < 1$. Looking at this curve as a function $\Phi_0 = \Phi_0(\mathcal{N})$, we observe that the polaron amplitude is a two-valued function of its norm. That is, equation (14) has two solutions for Φ_0 for all values of scaled norm ($\mathcal{N}$) satisfying $\mathcal{N} \leqslant \mathcal{N}_\mathrm{M}$, where $\mathcal{N}_\mathrm{M}$ is the maximum of the norm. However, due to the Vakhitov–Kolokolov [35] criterion, $\frac{\partial\mathcal{N}}{\partial\phi_0} > 0$, linearly stable polaron solutions, i.e. solutions stable with respect to longitudinal perturbations, may exist only for $\Phi_0 < \Phi_0^\mathrm{M}$. Here Φ_0^M denotes the position of the maximum of the curve $\mathcal{N}(\Phi_0)$. We found Φ_0^M and $\mathcal{N}_\mathrm{M}$, demanding $\frac{\partial\mathcal{N}}{\partial\Phi_0} = 0$, which yields

$$\Phi_0^\mathrm{M} \ln\left|\frac{1+\Phi_0^\mathrm{M}}{1-\Phi_0^\mathrm{M}}\right| = 2. \tag{15}$$

Combining the last equation and (14) we obtain

$$\mathcal{N}_\mathrm{M}\Phi_0^\mathrm{M} = 1. \tag{16}$$

Equation (15) has the following solution: $\Phi_0^\mathrm{M} \approx 0.835$ so that $\mathcal{N}_\mathrm{M} \approx 1.198$. In such a way, the above established large polaron stability condition reads

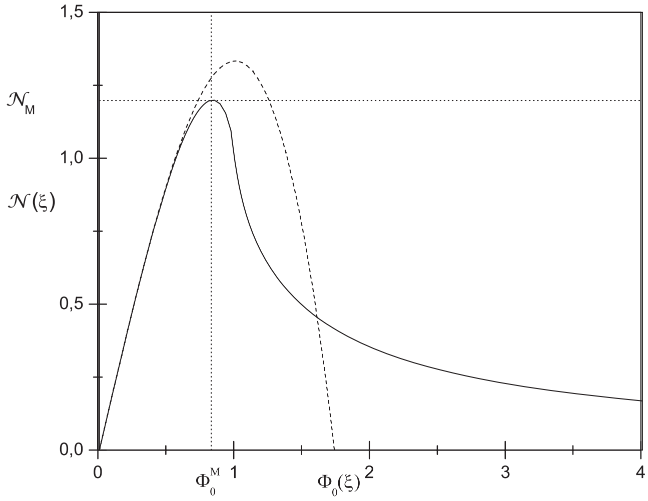

Figure 1. Scaled polaron norm $\mathcal{N}$ versus scaled amplitude Φ_0. The dotted line corresponds to an approximate cubic curve fitting well to the exact result in the limit $\Phi_0 \ll 1$.

$$\xi < 0.599\frac{J}{E_\mathrm{B}^0}. \tag{17}$$

It imposes the upper limit on the value of nonlocality parameter, over which an increase, for example due to a velocity increase, may destabilize the polaron. However, it may happen only for a comparably narrow polaron, since the applicability of the continuum approximation demands $\frac{2J}{E_\mathrm{B}^0} > 1$. Apart from this, violation of the above criterion takes place for very large values of nonlocality parameter which are outside the range of the approximation employed here.

In figure 2 we have plotted the polaron profile versus the coordinate in the moving frame whilst varying the nonlocality parameter for a few fixed values of the ratio $\frac{E_\mathrm{B}^0}{J}$. Evidently, for each particular value of this ratio the polaron profile has a typical bell-shaped form. The polaron amplitude and spatial extent are very sensitive to any change of this ratio: any rise of its magnitude results in a rise of the polaron amplitude followed by a reduction of its spatial extent. For each fixed value of E_B^0/J, the impact of nonlocality is manifested through a moderate amplitude increase and the shrinking of its spatial extent with a rise of ξ. The degree of these changes is pretty small with respect to the ones arising due to the modification of E_B^0/J. Nevertheless, the predicted effects may be quite significant for large values of this ratio which, however, cannot be arbitrarily large due to applicability of the continuum approximation, which demands $E_\mathrm{B}^0/2J \ll 1$. The decrease of this ratio reduces the impact of the nonlocality parameter so that predicted the effects become negligible for a very wide polaron ($E_\mathrm{B}^0/J \ll 1$). It may be more clearly seen from the explicit approximate expressions for the polaron amplitude and width

$$\phi_0 \approx \frac{E_\mathrm{B}^0}{\sqrt{2}J}\left[1 + \frac{1}{3}\left(\frac{E_\mathrm{B}^0}{J}\right)^2 \xi^2\right], \tag{18}$$

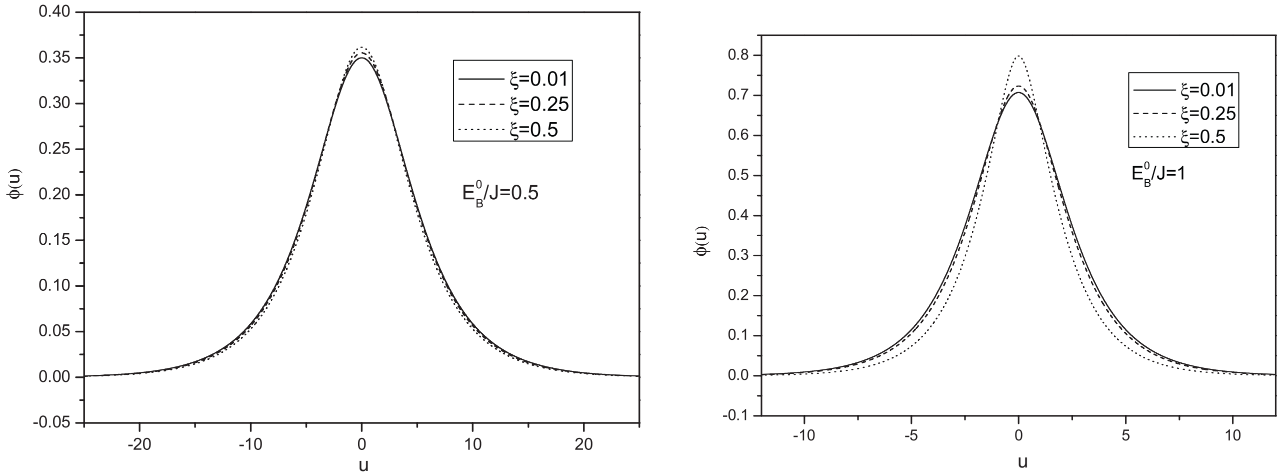

Figure 2. Polaron profile for a few different values of nonlocality parameter and ratio E^0_{B}/J.

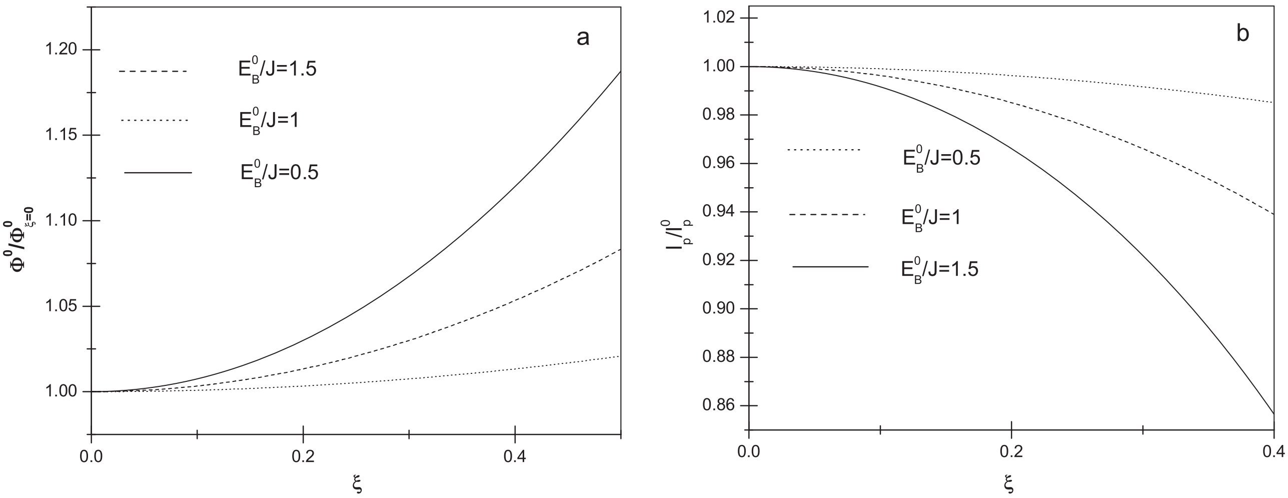

Figure 3. Polaron amplitude and width versus nonlocality parameter for a few different values of E^0_{B}/J.

$$l_{\mathrm{p}} \sim \sqrt{\int \left(\frac{x}{R_0}\right)^2 |\Psi(x)|^2 \frac{\mathrm{d}x}{R_0}} \approx l^0_{\mathrm{p}} \sqrt{1 - 0.74\left(\frac{E^0_{\mathrm{B}}}{J^2}\right)^2 \xi^2}. \tag{19}$$

Here $l^0_{\mathrm{p}} \sim \frac{\pi J}{\sqrt{2}E^0_{\mathrm{B}}}$ denotes the polaron width, in units of the lattice constant R_0, in the dispersionless limit. In deriving these expressions we exploited the fact that, as demonstrated in figure 1, for the region where a stable solution for the polaron amplitude appears, $\mathcal{N}(\xi)$ may be successfully approximated by the cubic function $\mathcal{N} \approx 2\Phi_0 - \frac{2}{3}\Phi_0^3$.

In figure 3 we plot (a) the polaron amplitude and (b) the width measured in units of lattice spacing as a function of nonlocality parameter for a few different values of the ratio E^0_{B}/J. The polaron width (amplitude) monotonically decreases (increases) with the nonlocality parameter. The degree of these changes must be estimated taking into account the applicability of the continuum approximation, which means that $E^0_{\mathrm{B}}/J < \frac{\pi}{\sqrt{2}}$. Decreasing this ratio enhances the validity of the continuum approximation but, as shown in figure 2, lowers the magnitude of the above predicted changes of polaron parameters which therefore become imperceptible for very large polarons.

5. Large polaron effective mass and ground state energy

We now focus on the evaluation of the large polaron energy, momentum and effective mass. This is of crucial importance for the understanding of the polaron dynamics, in particular the study of its mobility, in realistic conditions. Since the polaron is supposed to behave as a classical (Newtonian) particle we pursue the common procedure. It consists in the evaluation of the large polaron energy and momentum taking the expectation values of the operator of the total momentum $\hat{P}_{\mathrm{tot}} = \hat{P}_{\mathrm{e}} + \hat{P}_{\mathrm{ph}}$ and system Hamiltonian (1) in the trial state (2) within the continuum approximation. Then we evaluate the polaron effective mass by means of the relation $m_{\mathrm{eff}} = \frac{\partial P_{\mathrm{tot}}}{\partial v}|_{v=0}$. Here $\hat{P}_{\mathrm{e}} = \hbar \sum_k k A^\dagger_k A_k (A_k = \frac{1}{\sqrt{N}} \sum_n A_n \mathrm{e}^{\mathrm{i}knR_0})$ and $\hat{P}_{\mathrm{ph}} = \hbar \sum_q q b^\dagger_q b_q$ denote electron and

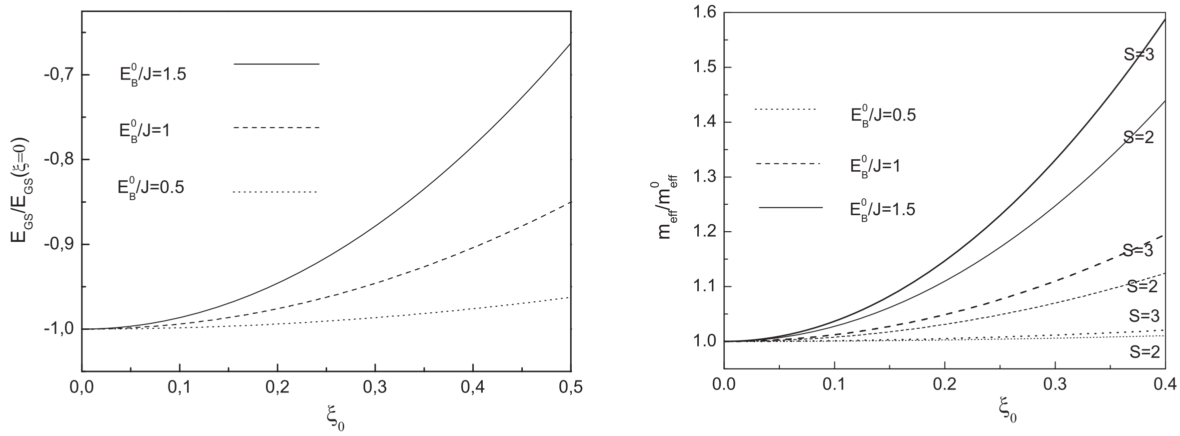

Figure 4. Polaron ground state energy and effective mass versus nonlocality parameter for different values of E_B^0/J and coupling constant.

phonon momentum, respectively. After some straightforward manipulations we obtain $P_{\text{tot}} = \frac{i\hbar}{2}(\int \frac{dx}{R_0}\Psi(x,t)\frac{\partial}{\partial x}\Psi^*(x,t) - \text{c.c.}) + \hbar\sum_q q|\beta_q|^2$, which, by virtue of equation (4), and together with the assumed form of electron wavefunction, attains the following form

$$P_{\text{tot}} = m^* v\left(1 + \frac{J^2}{2m^* E_B^0 \Omega_0^2 R_0^2} I(\xi, \phi_0)\right). \qquad (20)$$

In a similar way we obtain

$$E = \frac{m^* v^2}{2}\left(1 + \frac{J^2}{2m^* E_B^0 \Omega_0^2 R_0^2} I(\xi, \phi_0)\right) + \frac{J^2}{E_B^0} I'(\xi, \phi_0) - \frac{J^2}{2E_B^0} I''(\phi, \xi), \qquad (21)$$

where $I(\Phi_0, \xi) = 8\int_0^\infty dx\, \phi_x^2 \phi^2$, $I'(\xi, \phi_0) = 2\int_0^\infty dx\, \phi_x^2$, and $I''(\xi, \phi_0) = 2\int_0^\infty dx\, \phi^4 + I(\Phi_0, \xi)$. Their explicit expressions are given in the appendix.

The dependence of E on polaron momentum is given parametrically, through v, by equations (20) and (21), from which we easily find

$$v = \frac{\partial E}{\partial P_{\text{tot}}}, \qquad (22)$$

which proves that v is the polaron velocity.

Expanding the above integrals in powers of the small parameter and keeping only the leading order terms in ξ^2, we obtain approximate expressions for the polaron ground state energy ($E_{\text{GS}} \equiv E(v = 0)$) and effective mass.

$$E_{\text{GS}} \approx \left[-1 + \frac{3}{5}\left(\frac{E_B^0}{J}\right)^2 \xi_0^2\right] \frac{{E_B^0}^2}{12J}, \qquad (23)$$

$$m_{\text{eff}} \approx m_{\text{eff}}^0 \left\{1 + \frac{0.298 S^2 \xi_0^2 (\frac{E_B^0}{J})^4}{1 + 0.133 S^2 (\frac{E_B^0}{J})^2}\right\}. \qquad (24)$$

Here $\xi_0 \equiv \xi(v = 0)$, while $m_{\text{eff}}^0 = m^*[1 + (\frac{2SE_B^0}{15J})^2]$ denotes polaron effective mass in a dispersionless limit and coincides with the previously obtained one [2, 7, 8], which may be seen by expressing the coupling constant and adiabatic ratio in terms of the originally introduced parameters. Evidently, the polaron ground state energy and effective mass both increase monotonically with the nonlocality parameter.

In figures 2–4 we have plotted the dependence of the polaron amplitude, width, ground state energy and effective mass on the nonlocality parameter. We chose values of system parameters which satisfy the criteria for the existence of the large polaron. In general, the degree of the predicted changes depends substantially on the polaron radius i.e. ratio E_B^0/J. More precisely, the predicted effects are most significant for polarons which are not too large, and gradually vanish with a rise of polaron size. The most significant consequences could be for polaron effective mass, which may be considerably larger than that calculated without accounting for phonon dispersion. For the chosen set of system parameters the effective mass enhancement may go up to 15%. So large modification of the effective mass may affect the polaron dynamics substantially and, therefore, should be taken into account in the examination of polaron motion under the influence of external forces, in particular the electric field. In addition, polaron stability may be violated due to an increase of the ground state energy. Namely, the polaron, by definition, represents the most energetically favorable state. Therefore, its energy should be lower than the energy of free (band) states and condition $E_{\text{GS}} < 0$ must be satisfied. This yields the criterion for the energetic stability of the Holstein's large polaron

$$\xi_0 < 1.29\frac{E_B^0}{J}. \qquad (25)$$

Apparently, it is always satisfied provided that the linear stability condition (17) holds.

6. Concluding remarks

We have studied the motion of the Holstein's large polaron within the adiabatic approximation. This study in many respects differs from the previous ones [2, 7, 6]. In particular, the necessity of accounting for the phonon dispersion in the proper treatment of polaron motion is elaborated and taken into account explicitly. As a result we have derived the nonlocal nonlinear Schrödinger equation (NLNSE). It is solved in the weakly nonlocal limit $\xi \ll 1$, which reveals some unknown details of large polaron physics. In particular, we found that the polaron velocity and phonon dispersion have a substantial impact on the large polaron stability and values of its parameters. It is determined by the magnitude of the so called nonlocality parameter $\xi = \frac{\omega_1}{\sqrt{2}\omega_0}\sqrt{\frac{1+(v/c)^2}{1+(\omega_1/\omega_0)^2}}$. In particular, the polaron amplitude and effective mass increase, while its spatial extent decreases with a rise of nonlocality parameter. These effects are most significant for large value of E_B^0/J, a comparably narrow polaron, and vanish as it decreases.

Nonlocality effects are especially important for the polaron effective mass, whose gain may exceed 10%. It is determined by the magnitude of the ratio E_B^0/J. This indicates the necessity of accounting for the impact of these effects in the analysis of large polaron dynamics, for example mobility, in realistic conditions.

The predicted behavior of the large polaron effective mass as a function of the nonlocality parameter is quite the opposite of that of the nonadiabatic small polaron, which decreases with a rise of ω_1. In such a way, the intermolecular forces, which are the origin of the nonlocality effects, have a twofold role on the polaron features, depending on whether the quantum or classical nature of the phonon field prevails. In particular, these forces modify the character of the electron–phonon interaction, which becomes effectively long ranged: the electron located at the nth site of the molecular chain interacts with the molecule in the same site, directly, and indirectly, through these forces, with the neighboring ones. Consequently, a larger number of surrounding molecules are engaged in polaron formation and motion which, in certain circumstances, may result in an additional increase of its effective mass. On the other hand, an increase of ω_1 decreases the coupling constant and hardens the lattice which, therefore, became less deformable and less sensitive to the electron motion. In such a way, intermolecular forces may also have the opposite tendency and, in the final instance, may cause a decrease of the effective mass. These two opposite tendencies are balanced by the magnitude of ω_1 relative to J. Our results clearly showed that an increase of the effective mass as a function of nonlocality degree occurs in the adiabatic regime. Consequently, the opposite tendency should occur in the nonadiabatic regime. The physical grounds for such an expectation lies in the fact that an increase of ω_1 increases the maximal phonon frequency and violates the adiabatic condition and, in the final instance, may change the character of the dependence of the polaron parameter as a function of ω_1 or equivalently on nonlocality degree.

To prove the above expectations directly we refer to the seminal papers of Holstein [36] and Lang and Firsov [37], who demonstrated the exponential dependence (growth) of the small polaron effective mass as a function of the coupling constant: $m_{\mathrm{eff}}/m_0 \sim e^S$. As pointed out above, the inclusion of the phonon dispersion hardens the vibrational spectrum, decreases the coupling constant, which yields $S \sim \frac{S_0}{\sqrt{(1+(\omega_1/\omega_0)^2)^3}}$ (S_0 refers to the coupling constant in the absence of phonon dispersion), and leads to a decrease of the polaron effective mass as a function of the nonlocality degree.

Unfortunately, neither the semiclassical approach nor the usual small polaron theories can describe polaron behavior in the intermediate region and cannot precisely determine the values of the system parameters for which a particular tendency would prevail. We shall deal with this intriguing question in the subsequent article. However, in order to demonstrate the crucial role of the adiabatic parameter in that respect, we refer to the more sophisticated approaches [19, 18] for the evaluation of m_{eff}. These methods yield a slightly more complicated expression for the effective mass ($m_{\mathrm{eff}}/m_0 \sim \mathrm{e}^{f(B,S,\xi;\mathrm{e}^{-f})}$), in which the band narrowing factor $f(B, S, \xi; \mathrm{e}^{-f})$ is defined through a self-consistent relation. However, as far as the nonadiabatic condition is satisfied, the effective mass qualitatively displays the same behavior as predicted by the Holstein and Lang–Firsov approaches. An increase of the adiabatic ratio reduces the band narrowing factor, which becomes negligible in the adiabatic limit $2J \gg \hbar\Omega$.

A particularly interesting aspect concerns the impact of the nonlocality on polaron stability. In that respect we recall that in the dispersionless phonon Holstein model large polaron dynamics is described within the local cubic nonlinear NSE. Its exact integrability automatically provides the extreme stability of polaron solutions with respect to external perturbations (linear stability). That is, provided that the aforementioned basic assumptions for large polaron existence–adiabatic strong coupling limit and applicability of continuum approximation–are satisfied, the large polaron is always stable for any values of system parameters. Quite to the contrary, due to the inclusion of phonon dispersion the integrable NSE is replaced by its nonintegrable counterpart, which imposes certain restrictions on the allowed values of system parameters. In particular, linearly stable polaron solutions may appear only for $\frac{E_B^0}{J} < \frac{0.599}{\xi}$.

Let us finally comment on the impact of the polaron velocity on its properties. In particular, an increase of polaron velocity enlarges the degree of nonlocality and consequently modifies the soliton parameters, both the amplitude and width, and, in the final instance, may destabilize polaron. This is quite similar to the dependence of these parameters on polaron velocity, as in the case of the acoustic polaron. In the present case these effects are not so important and range up to a few per cent only. Moreover, due to the above established stability criterion, the polaron velocity cannot exceed the critical value $v_c = \sqrt{v_M^2 - c^2}$. Here $v_M = 0.36\Omega_0 R_0 (J/E_B^0)$ represents the maximal velocity of a large polaron in the dispersionless limit. It is substantially less than the minimal phase velocity of optic phonons, which Wilson [6] conjectured as that supposed to be the maximal velocity which Holstein's large polaron may attain. Otherwise, a catastrophe would appear in the large polaron parameters when its velocity approaches the minimum optic phonon phase velocity. Our analysis suggests that the gradual change of the polaron parameters and its destabilization due to an increase of velocity must emerge long before this catastrophe can arise.

To date the influence of the phonon dispersion and velocity on large polaron properties in the adiabatic limit has not been taken into account within Holstein's model. In particular, to the best of our knowledge, the influence of the polaron velocity on polaron properties was only considered in Wilson's paper [6], but without taking into account the phonon dispersion. Therefore, no quantitative comparison is possible with the present results. However, in comparison with the related problem, the motion of the Fröhlich large polaron, we obtain the analogous results concerning the influence of the phonon dispersion on polaron stability. Quite to the contrary, the effective mass of the Fröhlich large polaron decreases with an increase of the phonon group velocity. This effect is the consequence of the very different low dispersion ($\omega_q = \sqrt{\omega_0^2 + u^2q^2}$, where u is the group velocity) of the polar optical phonons participating in Fröhlich large polaron creation.

In conclusion we emphasize that our analysis indicates that one should treat the problem of large adiabatic polaron motion much more caution than before. In particular, the inclusion of phonon dispersion and the explicit dependence of the polaron parameters on its velocity are necessary. Considerable effects are expected for polaron kinetic parameters, for example mobility, which implies the importance of the present results in the interpretation of the experimental data concerning charge and energy transfer in realistic media.

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Appendix

$$I(\Phi_0, \xi) = \frac{1}{32\sqrt{2}\xi^5}\left\{3\xi\phi_0 - 2\xi^3\phi_0^3 + \frac{1}{2\sqrt{2}}(4\xi^4\phi_0^4 + 4\xi^2\phi_0^2 - 3)\ln\left|\frac{1+\sqrt{2}\xi\phi_0}{1-\sqrt{2}\xi\phi_0}\right|\right\},$$

$$I(\Phi_0, \xi) \approx \frac{2\phi_0^5}{15\sqrt{2}}\left[1 + \frac{4}{7}\xi^2\phi_0^2\right]. \tag{26}$$

$$I'(\Phi_0, \xi) = \frac{\phi_0}{4\sqrt{2}\xi^2} - \frac{(1-2\xi^2\phi_0^2)}{16\xi^3}\ln\left|\frac{1+\sqrt{2}\xi\phi_0}{1-\sqrt{2}\xi\phi_0}\right|,$$

$$I'(\Phi_0, \xi) \approx \frac{\phi_0^3}{3\sqrt{2}}\left[1 + \frac{2}{5}\xi^2\phi_0^2\right], \tag{27}$$

$$I''(\Phi_0, \xi) = \frac{\sqrt{2}\phi_0}{16\xi^2}(1 - 6\xi^2\phi_0^2) - \frac{1}{32\xi^3}(1-2\xi^2\phi_0^2)(1+6\xi^2\phi_0^2)\ln\left|\frac{1+\sqrt{2}\xi\phi_0}{1-\sqrt{2}\xi\phi_0}\right|$$

$$I''(\Phi_0, \xi) \approx \frac{2\sqrt{2}}{3}\left(1 - \frac{4}{5}\phi_0^2\xi^2\right)\phi_0^3. \tag{28}$$

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