The motion of an excess electron in a molecular chain when the interaction with optical phonons is taken into account

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We show that the motion, in a molecular chain, of an excess electron that interacts with nondipolar optical and electrically dipolar phonons is accompanied by a local deformation of the chain. When the electron velocity increases to its critical value, the localization region caused by the interaction with the nondipolar optical phonons decreases; when its velocity increases further the electron starts to get delocalized. If the localization of the electon is caused by its nonlocal interaction with the electrically dipolar phonons, increasing the electron velocity makes its localization difficult even at low velocities.

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1. INTRODUCTION

In Refs. 1 to 3 the effect of acoustic phonons with dispersion

$$\Omega_{ac}(k)=kV_{ac} \tag{1.1}$$

on the motion of an excess electron (or exciton) in a one-dimensional molecular chains was studied. Without using the adiabatic approximation or perturbation theory in the interaction force, it was shown that the steady motion of an electron (exciton) with velocities below the group velocity of longitudinal sound is accompanied by a local deformation of the chain. This motion is described by a solitary wave which does not change its shape and velocity and which is called a soliton. For velocities above the sound speed there are no soliton solutions. The motion of the electron (exciton) is described by a spreading wave packet and is retarded due to the emission of phonons.

In the present paper we study, without using the adiabatic approximation or perturbation theory, the effect of optical non-dipolar and electrically dipolar and electrically dipolar phonons with dispersion

$$\Omega^2(k)=\Omega_0^2+k^2V_0^2 \tag{1.2}$$

on the motion of an excess electron. In (1.2) V_0 corresponds to only the minimum phase velocity of the optical phonons, so that the motion of the electron can be accompanied by a deformation also at velocities above V_0.

We consider as our model a one-dimensional chain formed of identical molecules at a distance a from one another and possessing constant dipole moments which are directed along the chain. Such a system is, in particular, a model for the α-spiral protein molecule in which the peptide groups ("molecules") are maintained at distances of 4.5 Å from one another by hydrogen bonds, forming three quasi-periodic chains. Each peptide group has a constant electrical dipole moment which is approximately equal to 4 Debye. Protein molecules can transfer electrons from donors to acceptors so that the study of the nature of the motion of an excess electron in quasi-one-dimensional molecular chains is of considerable interest.

2. EQUATIONS OF MOTION FOR AN ELECTRON INTERACTING WITH NON-DIPOLAR PHONONS

Turner and Anderson[4] have evaluated the ground state energy and the wave functions of an electron in the field of an isolated electrical dipole. The overlapping of the electron wave functions in a chain formed by periodically spaced molecules with constant dipole moments leads to a collectivation of electron states. An excess electron having arrived in such a chain from a donor is described in the effective-mass (m) approximation by the Hamiltonian

$$H_{el}=\frac{1}{a}\int\Psi^*(x,t)\left(\mathscr{E}_0-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\Psi(x,t)\,dx, \tag{2.1}$$

where $\mathscr{E}_0$ is the energy of the bottom of the conduction band and $\Psi(x,t)$ the wave function normalized by the condition[1)]

$$\frac{1}{a}\int|\Psi(x,t)|^2\,dx=1\,. \tag{2.2}$$

Let $u_n(t)$ be the displacement, which determines the longitudinal optical oscillation branch, of the atoms in the n-th molecule. If the displacements $u_n(t)$ are not connected with a change in the intrinsic constant dipole moments of the molecules, then their interaction with the electron is determined by the local deformation potential, which in the continuum approximation is given in the form

$$H_{int}=\frac{\chi}{a}\int|\Psi(x,t)|^2u(x,t)\,dx, \tag{2.3}$$

where x/a is the number of the site of the chain in the continuum approximation while χ is the interaction parameter.

If Ω_0 is the frequency of the intramolecular oscillations, the optical phonons in the chain with dispersion (1.2) are described by the Hamiltonian

$$H_{ph}=\frac{M}{2a}\int\left[\left(\frac{\partial u}{\partial t}\right)^2+\Omega_0^2u^2+V_0^2\left(\frac{\partial u}{\partial x}\right)^2\right]dx, \tag{2.4}$$

where M is the reduced mass of the atoms responsible

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for the intramolecular vibration.

Regarding the expression

$$H=H_{el}+H_{ph}+H_{int} \tag{2.5}$$

as the Hamiltonian of an electron interacting with the optical phonons, we get the equations of motion

$$\frac{\partial^2 u}{\partial t^2}+\Omega_0^2u-V_0^2\frac{\partial^2 u}{\partial x^2}+\frac{\chi}{M}|\Psi|^2=0, \tag{2.6}$$

$$i\hbar\frac{\partial\Psi}{\partial t}-\mathscr{E}_0\Psi+\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}-\chi u\Psi=0. \tag{2.7}$$

Because of the translational symmetry of the system we can look for the solutions of Eqs. (2.6) and (2.7) in the form of excitations that propagate along the chain with a constant velocity V. To do this we use the equations

$$u(x,t)=u(\xi),\quad \Psi(x,t)=\varphi(\xi)\exp\left\{\frac{i}{\hbar}\left[mVx-\left(\Lambda+\mathscr{E}_0+\frac{1}{2}mV^2\right)t\right]\right\} \tag{2.8}$$

to introduce functions $u(\xi)$ and $\varphi(\xi)$ which depend on the dimensionless variable

$$\xi=(x-x_0-Vt)/a. \tag{2.9}$$

From Eq. (2.6) it then follows that[2]

$$u(\xi)=-\frac{\chi}{M\Omega_0^2}\int d\xi_1\,w(\xi-\xi_1)\varphi^2(\xi_1), \tag{2.10}$$

$$w(\xi)=\frac{1}{2\pi}\int\frac{e^{iq\xi}dq}{1+\varepsilon q^2}=\begin{cases}\frac{1}{2}\varepsilon^{-1/2}\exp\left(-\frac{|\xi|}{\varepsilon^{1/2}}\right), & \text{if}\quad \varepsilon>0; \quad (2.11\text{a})\\ \delta(\xi), & \text{if}\quad \varepsilon=0; \quad (2.11\text{b})\\ \frac{\theta(-\xi)}{(-\varepsilon)^{1/2}}\sin\frac{|\xi|}{(-\varepsilon)^{1/2}}, & \text{if}\quad \varepsilon<0. \quad (2.11\text{c})\end{cases}$$

Here

$$\theta(\xi)=\begin{cases}1, & \text{if}\quad \xi>0,\\ 0, & \text{if}\quad \xi<0:\end{cases}\qquad \varepsilon=\frac{V_0^2-V^2}{a^2\Omega_0^2}. \tag{2.12}$$

According to (2.10) the function $w(\xi)$ takes into account the fact that the interaction of the electron with the non-dipolar optical phonons is not local, because of the influence of their spatial dispersion ($V_0\neq 0$) and because of the retardation time due to the electron motion ($V\neq 0$). The two effects partially cancel each other so that when $V=V_0$ the function $w(\xi)$ is transformed into the delta-function (2.11b). For very small electron speeds ($V<V_0$) the effect of the spatial dispersion dominates and the function (2.11a) is symmetric under a change in sign of ξ. At velocities V larger than V_0 the time retardation dominates. According to (2.11c) only the regions $\xi_1<\xi$ contribute therefore to the integral (2.11).

Substituting (2.8) and (2.10) into Eq. (2.7) we get the integro-differential equation

$$\left(\frac{\hbar^2}{2ma^2}\frac{d^2}{d\xi^2}+\Lambda+\frac{\chi}{M\Omega_0^2}\int d\xi_1 w(\xi_1-\xi)\varphi^2(\xi_1)\right)\varphi(\xi)=0. \tag{2.13}$$

The electron states described by the localized solutions of Eq. (2.13) and satisfying the normalization condition

$$\int\varphi^2(\xi)d\xi=1, \tag{2.14}$$

will be called electro-solitons.

Knowing the solution of Eq. (2.13) we can use Eq. (2.10) to evaluate the function $u(\xi)$ of the intramolecular displacements which accompany the motion of the electron, and also two integrals of motion—the total energy

$$E(V)=\mathscr{E}_0+\frac{1}{2}mV^2+\int\varphi\left(\chi u\varphi-\frac{\hbar^2}{2ma^2}\frac{d^2\varphi}{d\xi^2}\right)d\xi + \frac{M\Omega_0^2}{2}\int\left[\frac{(V^2+V_0^2)}{a^2\Omega_0^2}\left(\frac{du}{d\xi}\right)^2+u^2\right]d\xi \tag{2.15}$$

and the total momentum

$$P(V)=\left(m+\frac{M}{a^2}\int\left(\frac{du}{d\xi}\right)^2d\xi\right)V. \tag{2.16}$$

3. APPROXIMATION OF SMALL ELECTRO-SOLITON VELOCITIES

In molecular lattices the inequality $V_0^2\ll a^2\Omega_0^2$ is usually satisfied so that for low velocities $V\sim V_0$ we have according to (2.12) $|\varepsilon|\ll 1$. In this case the kernel $w(\xi)$ of Eq. (2.13) can be written in the form

$$w(\xi)=\delta(\xi)+\varepsilon\frac{d^2}{d\xi^2}\delta(\xi), \tag{3.1}$$

and the equation itself reduces to the stationary modified non-linear Schrödinger equation[5-7]

$$\frac{d^2\varphi}{d\xi^2}+4\alpha\varphi^3+4\alpha\varepsilon\varphi\frac{d^2\varphi^2}{d\xi^2}-\lambda^2\varphi=0 \tag{3.2}$$

with the following dimensionless parameters

$$\alpha=\frac{ma^2\chi^2}{2\hbar^2\Omega_0^2M},\quad \lambda^2=-\frac{2ma^2}{\hbar^2}\Lambda. \tag{3.3}$$

Equation (3.2) has an exact soliton solution

$$\xi=\frac{1}{2\lambda}\ln\frac{|A^{1/2}-B^{1/2}|}{A^{1/2}+B^{1/2}}+|\varepsilon|^{1/2}C, \tag{3.4}$$

$$A=1+8\alpha\varepsilon\varphi^2,\quad B=1-2\alpha\varphi^2/\lambda^2, \tag{3.4a}$$

$$C=\begin{cases}2\,\mathrm{arctg}(A/4\varepsilon\lambda^2B)^{1/2}, & \text{if}\quad \varepsilon\geqslant 0;\\ \ln\frac{|A^{1/2}-(4|\varepsilon|\lambda^2B)^{1/2}|}{A^{1/2}+(4|\varepsilon|\lambda^2B)^{1/2}}, & \text{if}\quad \varepsilon<0.\end{cases} \tag{3.4b}$$

When $\varepsilon=0$ Eq. (3.2) reduces to the stationary nonlinear Schrödinger equation. Its solution, normalized by condition (2.14) can be obtained from (3.2) for the value $\varepsilon=0$. In that case $\lambda=\pm\alpha$ and

$$\varphi(\xi)=(\alpha/2)^{1/2}\,\mathrm{ch}^{-1}\alpha\xi.$$

Hence the region where the soliton is localized $[\varphi(\xi)\leq 0.1\varphi(0)]$ in the chain is determined by the expression

$$\Delta x\approx 2a\pi/\alpha. \tag{3.5}$$

The continuum approximation is thus justified for parameter values $\alpha<2\pi$.

When $\varepsilon\neq 0$ but satisfies the inequality

$$8\alpha|\varepsilon|\varphi^2\ll 1, \tag{3.6}$$

it follows from (3.4) that

$$\xi\approx\frac{1}{2\lambda}\ln\frac{(1-B^{1/2})(1-4\varepsilon\lambda^2B^{1/2})}{1+B^{1/2}}. \tag{3.7}$$

Solving (3.7) for φ^2 we find, up to terms of order $(\varepsilon\lambda^2)^2$,

$$\varphi^2(\xi)=\frac{\lambda^2}{2\alpha}\mathrm{ch}^{-2}\lambda\xi(1+4\varepsilon\lambda^2\,\mathrm{th}^2\lambda\xi). \tag{3.8}$$

It then follows from the normalization condition (2.14) that

$$\lambda=\pm\alpha\left(1-\frac{4}{3}\varepsilon\alpha^2\right). \tag{3.9}$$

Using Eqs. (2.10), (3.1), and (3.8) we find the function which determines the intramolecular displacements:

$$u(\xi)=-\frac{\chi\lambda^2}{2\alpha M\Omega_0^2}\operatorname{ch}^{-2}\lambda\xi[1+2\varepsilon\lambda^2(4-5\operatorname{ch}^{-2}\lambda\xi)]. \tag{3.10}$$

Furthermore we can use Eqs. (2.15) and (2.16) to evaluate the energy $E(V)$ and momentum $P(V)$ of the electro-soliton which propagates with a constant velocity V. Up to terms of order ε^2 they are determined by the expressions

$$E(V)=E(0)+\frac{1}{2}m_{\text{sol}}V^2, \tag{3.11}$$

$$P(V)=m_{\text{sol}}V, \tag{3.12}$$

where

$$m_{\text{sol}}=m\left(1+\frac{8\hbar^2\alpha^4}{15a^4m^2\Omega_0^2}\right), \tag{3.13}$$

$$E(0)=\mathscr{E}_0-\Delta,\quad \Delta=\frac{\hbar^2\alpha^2}{6ma^2}\left(1-\frac{8\alpha^2V_0^2}{5a^2\Omega_0^2}\right). \tag{3.14}$$

According to (3.8) and (3.10) the electro-soliton localization region

$$\Delta x\approx 2\pi a/\alpha\left(1-\frac{4}{3}\varepsilon\alpha^2\right)$$

decreases with increasing velocity V.

The solutions $\varphi(\xi)$ of Eq. (2.13), corresponding to the smallest Λ, can also be found in the approximation (3.1) through minimizing the functional

$$J\{\varphi\}=-\frac{\hbar^2}{2ma^2}\int d\xi\,\varphi(\xi)\left(\frac{d^2\varphi}{d\xi^2}+2\alpha\varphi\left(\varphi^2+\varepsilon\frac{d^2\varphi^2}{d\xi^2}\right)\right) \tag{3.15}$$

with the normalization condition (2.14). The functional (3.15) with the normalized trial function

$$\varphi(\xi)=(\gamma/2)^{1/2}\operatorname{ch}^{-1}\gamma\xi, \tag{3.16}$$

which depends on one variational parameter becomes a cubic polynomial

$$J(\gamma)=\frac{\hbar^2}{3ma^2}\left(\frac{4}{5}\varepsilon\alpha\gamma^3+\frac{1}{2}\gamma^2-d\gamma\right)$$

the minimum of which is reached for the value

$$\gamma=\gamma_0=\alpha\left(1-\frac{12}{5}\varepsilon\alpha^2\right). \tag{3.17}$$

Evaluating futher the total energy $E(V)$ and momentum $P(V)$ of the electro-soliton we find again (accurate to ε^2) expressions (3.11) and (3.12) with the values (3.13) and (3.14).

4. ELECTRO-SOLITON WITH VELOCITIES $V\gg V_0$

For velocities $V\gg V_0$ such that $V^2\sim a^2\Omega_0^2$, $|\varepsilon|$ is of order unity. In that case it is impossible to use the approximate Eq. (3.1) and it is necessary to solve Eq. (2.13) with the kernel of the integral operator (2.11c):

$$\left(\frac{\hbar^2}{2ma^2}\frac{d^2}{d\xi^2}+\Lambda+\frac{\chi^2}{M\Omega_0^2}\int d\xi_1\,\varphi^2(\xi_1)\frac{\theta(\xi_1-\xi)}{|\varepsilon|^{1/2}}\sin\frac{|\xi-\xi_1|}{|\varepsilon|^{1/2}}\right)\varphi(\xi)=0. \tag{4.1}$$

As the exact solutions of Eq. (4.1) are not known we calculate $\varphi(\xi)$ corresponding to the smallest value of Λ by a direct variational method, using the functional

$$J\{\varphi\}=-\frac{\hbar^2}{2ma^2}\left(\int d\xi\,\varphi(\xi)\frac{d^2\varphi}{d\xi^2}\right.$$
$$\left.-2\alpha\int d\xi\int d\xi_1\,\varphi^2(\xi_1)\frac{\theta(\xi_1-\xi)}{|\varepsilon|^{1/2}}\sin\frac{|\xi_1-\xi|}{|\varepsilon|^{1/2}}\varphi^2(\xi)\right). \tag{4.2}$$

The trial function

$$\varphi(\xi)=(\rho^2/\pi)^{1/4}\exp(-\rho^2\xi^2/2), \tag{4.3}$$

which depends on one variational parameter ρ, reduces the variational problem to finding the minimum of the function

$$J(\rho)=\frac{\hbar^2}{2ma^2}F(\rho),\quad F(\rho)=\frac{\rho^2}{2}+\frac{i\alpha}{|\varepsilon|^{1/2}}\Phi(z)e^{z^2}, \tag{4.4}$$

where the variable is $z=i(2\rho^2|\varepsilon|)^{-1/2}$ while

$$\Phi(z)=\frac{2}{\sqrt{\pi}}\int_0^z e^{t^2}dt$$

is the probability function.

For large $|z|$ (the case of small $\rho^2|\varepsilon|$) we get, using the asymptotic expansion for $\Phi(z)$ (see, for instance, Ref. 8, Eq. 7.1.23), after some transformations, up to terms of order ρ^6,

$$F(\rho)={}^1/_2\rho^2+\rho_0(\varepsilon\rho^3-\rho),\quad \rho_0=\alpha(2/\pi)^{1/2}. \tag{4.5}$$

The minimum of the function (4.5) is reached for the value

$$\rho_1=\rho_0(1-3\varepsilon\rho_0^2)\quad(|\varepsilon|\rho^2\ll 1,\ \varepsilon<0). \tag{4.6}$$

In that case

$$\Lambda=J(\rho_1)=-\frac{\hbar^2\rho_0^2}{4ma^2}(1-2\varepsilon\rho_0^2).$$

When the inequality $\rho^2|\varepsilon|\ll 1$ is satisfied, it thus follows from Eq. (4.6) that when the velocity increases the size of the electro-soliton diminishes.

The energy and momentum of the electro-soliton are given by Eqs. (3.11) and (3.12) with the values

$$E(0)=\mathscr{E}_0-\Delta,\quad \Delta=\hbar^2\alpha^2/2\pi ma^2, \tag{4.7}$$

$$m_{\text{sol}}=m\left(1+\frac{4\alpha^4\hbar^2}{\pi^2a^4m^2\Omega_0^2}\right). \tag{4.8}$$

If the inequality $\rho^2|\varepsilon|\ll 1$ is not satisfied, we can transform Eq. (4.4) into

$$F(\rho)=\frac{1}{2}\rho^2-\frac{2\alpha}{(\pi|\varepsilon|)^{1/2}}D\left(\frac{1}{x}\right), \tag{4.9}$$

where $x=(2|\varepsilon|)^{1/2}\rho$, while

$$D\left(\frac{1}{x}\right)=\exp\left(-\frac{1}{x^2}\right)\int_0^{1/x}\exp t^2\,dt$$

is the Dawson integral.[8] The value of ρ which minimizes the function $F(\rho)$ is the root of the equation

$$x^4/2x_0+x=2D(1/x), \tag{4.10}$$

where $x_0=\rho_0(2|\varepsilon|)^{1/2}$. Numerically solving Eq. (4.10) we find the function $x/x_0=\rho/\rho_0$, which is shown in the figure.

It follows from the figure that when $x_0<0.1$, the function x/x_0 is described by Eq. (4.6). When $0<x_0<0.304$ the function x/x_0 increases, which corresponds to a decrease in the size of the electro-soliton. After reaching its maximum value, 1.643 at $x_0=0.304$, which corresponds to the critical velocity

$$V_{\text{cr}}\approx 0.3\pi^{1/2}M\hbar^2\Omega_0^3/ma\chi^2, \tag{4.11}$$

the function x/x_0 decreases when the velocity is further increased, corresponding to a delocalization of the electron.

When the interaction between the electron and the non-dipolar optical phonons is taken into account, the velocity-dependence of the size of the electro-soliton has thus a different character from that in the case of the interaction of the electron with acoustical phonons.[1-3] The instability of the soliton is determined by the magnitude of the energy gap Δ [see (3.14), (4.7)].

5. INTERACTION BETWEEN THE ELECTRON AND ELECTRIC DIPOLE PHONONS

The interaction with all the constant electric dipole moments of the molecules of the chain is taken into account in the operator (2.1). If the displacements $u_n(t)$ are connected with a change in the electric dipole moments, their additional interaction with the electron has a non-local character. In the continuum approximation it is given by the expression

$$H_{int}=\frac{e^2}{\tilde{\varepsilon}a}\int dx\int_a^\infty\frac{dy}{y^2}\,(u(x+y,t)+u(x-y,t))\,|\Psi(x,t)|^2, \tag{5.1}$$

where e is some effective charge, $\tilde{\varepsilon}$ the effective permittivity introduced by Pekar[9] and takes into account the inertial polarizability of the molecules ($1/\tilde{\varepsilon}=0.1$ to 0.3).

The equations of motion of the system described by the sum of the Hamiltonians (2.1), (2.4), and (5.1) have the form

$$\frac{\partial^2u}{\partial t^2}+\Omega_0^2u-V_0^2\frac{\partial^2u}{\partial x^2}+\frac{e^2}{\tilde{\varepsilon}aM}\int_a\frac{dy}{y^2}\,(|\Psi(x-y,t)|^2+|\Psi(x+y,t)|^2)=0, \tag{5.2}$$

$$i\hbar\frac{\partial\Psi}{\partial t}-\mathscr{E}_0\Psi+\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}-\frac{e^2}{\tilde{\varepsilon}a}\Psi\int_a^\infty\frac{dy}{y^2}\,(u(x+y,t)+u(x-y,t))=0. \tag{5.3}$$

Using Eq. (2.8) to change to the real functions $u(\xi)$ and $\varphi(\xi)$, we get from Eq. (5.2)

$$u(\xi)=\frac{e^2}{\tilde{\varepsilon}M\Omega_0^2a^2}\int d\xi_1\int_1^\infty\frac{d\xi_2}{\xi_2^2}\,w(\xi_1-\xi)\,(\varphi^2(\xi_1-\xi_2)+\varphi^2(\xi_1+\xi_2)), \tag{5.4}$$

where $w(\xi)$ is determined by Eq. (2.11).

Substituting (5.4) and (2.8) in Eq. (5.2) we find the integro-differential equation

$$\left(\frac{\hbar^2}{2ma^2}\frac{d^2}{d\xi^2}+\Lambda+\frac{e^4}{\tilde{\varepsilon}^2M\Omega_0^2a^4}\int_1^\infty\frac{d\xi_2}{\xi_2^2}\int_1^\infty\frac{d\xi_3}{\xi_3^2}\int d\xi_1\,w(\xi-\xi_1)\right.$$
$$\left.\times\sum_{k,l=\pm1}\varphi^2(\xi_1+k\xi_2+l\xi_3)\right)\varphi(\xi)=0. \tag{5.5}$$

We determine the solution of Eq. (5.5) corresponding to the lowest value of Λ by varying the functional

$$J\{\varphi\}=\frac{\hbar^2}{2ma^2}\left[\int d\xi\left(\frac{d\varphi}{d\xi}\right)^2\right.$$
$$\left.-G\int d\xi\int d\xi_1\int_1^\infty\frac{d\xi_2}{\xi_2^2}\int_1^\infty\frac{d\xi_3}{\xi_3^2}\varphi^2(\xi)\,w(\xi-\xi_1)\sum_{k,l=\pm1}\varphi^2(\xi_1+k\xi_2+l\xi_3)\right] \tag{5.6}$$

under the additional condition (2.14) and at the value

$$G=me^4/\tilde{\varepsilon}^2Ma^2\hbar^2\Omega_0^2. \tag{5.7}$$

When $|\varepsilon|\ll1$ we can use in the functional (5.6) the approximate Eq. (3.1). We then have

$$J\{\varphi\}=\frac{\hbar^2}{2ma^2}\left[\int d\xi\left(\frac{d\varphi}{d\xi}\right)^2-G(I_1(\varphi)+\varepsilon I_2(\varphi))\right], \tag{5.8}$$

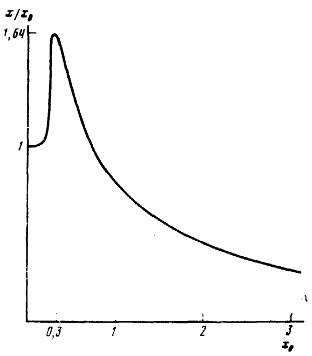

FIG. 1. The coordinates are $x_0=(2|\varepsilon|)^{1/2}\rho_0$ and $x/x_0=\rho/\rho_0$. The maximum value 1.643 is reached at $x_0=0.304$.

$$I_1(\varphi)=\int d\xi\int_1^\infty\frac{d\xi_2}{\xi_2^2}\int_1^\infty\frac{d\xi_3}{\xi_3^2}\varphi^2(\xi)\sum_{k,l=\pm1}\varphi^2(\xi+k\xi_2+l\xi_3), \tag{5.9}$$

$$I_2(\varphi)=\int d\xi\int_1^\infty\frac{d\xi_2}{\xi_2^2}\int_1^\infty\frac{d\xi_3}{\xi_3^2}\frac{d^2\varphi^2(\xi)}{d\xi^2}\sum_{k,l=\pm1}\varphi^2(\xi+k\xi_2+l\xi_3). \tag{5.10}$$

Applying the straight variational method and the trial function (4.3) we get after some calculations up to quantities of the order ρ^4

$$I_1\approx2(2/\pi)^{1/2}\rho-4\rho^2,\quad I_2\approx8\pi^{-1/2}\rho^2\quad(\rho\ll\sqrt{2}). \tag{5.11}$$

After substituting (5.11) and (4.3) into (5.8) we get the function

$$J(\rho)=\frac{h^2}{2ma^2}\left[\frac{1}{2}\rho^2-G\rho\left(2\left(\frac{2}{\pi}\right)^{1/2}-4\rho(1-2\varepsilon\pi^{-1/2})\right)\right],$$

the minimum of which, $\Lambda=J(\rho_1)$, is reached for the value

$$\rho_1=\frac{2G(2/\pi)^{1/2}}{1+8G(1-2\varepsilon/\pi)}\approx\rho_0(1+2^{3/2}\rho_0\varepsilon), \tag{5.12}$$

where $\rho_0=2G(2/\pi)^{1/2}/(1+8G)$ is the parameter determining the size of the electro-soliton $\varepsilon=0$. When the non-linearity parameter (5.7) changes within the limits 0.1 to 10, ρ_0 increases monotonically within the limits 0.09 to 0.20.

It follows from Eqs. (5.12) and (2.12) that when $|\varepsilon|\ll1$ and values of $G\leqslant10$ for which our approximation ($\rho\ll\sqrt{2}$) is justified, the size of the electro-soliton increases with increasing velocity.

Using the explicit form of the function (4.3) we get the function

$$u(\xi)=\frac{2e^2\rho_1}{\tilde{\varepsilon}\sqrt{\pi}\,a^2M\Omega_0^2}\left(1+\varepsilon\frac{d^2}{d\xi^2}\right)\exp(-\rho_1^2\xi^2).$$

The energy $E(V)$ of the electro-soliton is given by (3.11) with the values

$$E(0)=\mathscr{E}_0-\Delta,\qquad\Delta=\frac{\hbar^2G\rho_0}{(2\pi)^{1/2}ma^2}\left(1+4\sqrt{2}\frac{V_0^2\rho_0}{a^2\Omega_0^2}\right),$$
$$m_{sol}=m\left(1+\frac{16\hbar^2\rho_0^2G}{\pi^{1/2}m^2a^4\Omega_0^2}\right).$$

The total momentum is given by the expression

$$P(V)=m_{sol}^1V$$

for the value

$$m_{sol}^1=m\left(1+\left(\frac{8}{\pi}\right)^{1/2}\frac{\hbar^2\rho_0^3G}{m^2a^4\Omega_0^2}\right).$$

[1] Unless otherwise stipulated, the integrations in Eqs. (2, 1), (2.2) and in all subsequent equations is between infinite limits.

[2] When $\varepsilon < 0$ the circuit around the poles of the integrand in (2.11) is given by the rule

$$w(\xi)=\lim_{\delta\to 0}\int_{-\infty}^{\infty}\frac{e^{iq\xi}\,d\xi}{1+\varepsilon(q+i\delta)^2}.$$

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[1] A. S. Davydov, Teor. Mat. Fiz. **40**, 408 (1979).

[2] A. S. Davydov, Zh. Eksp. Teor. Fiz. **78**, 789 (1980) [Soviet Phys. JETP **51**, 397 (1980)].

[3] A. S. Davydov, Int. J. Quantum Chem. **16**, 5 (1979).

[4] I. E. Turner V. E. Anderson, and K. Fox, Phys. Rev, **174**, 81 (1968).

[5] I. V. Simenog, Teor. Mat. Fiz. **30**, 408 (1977).

[6] A. Makamura, J. Phys. Soc. Japan **42**, 1824 (1977).

[7] A. G. Litvak and A. M. Sergeev, Pis'ma Zh. Eksp. Teor. Fiz. **27**, 549 (1978) [JETP Lett. **27**, 517 (1978)].

[8] M. Abramowitz and I. A. Stegun, Handbook of Mathematical Functions, Dover, New York, 1965.

[9] S. I. Pekar, Issledovaniya po elektronnoĭ teorii kristallov (Studies of the electron theory of crystals) Gostekhizdat, Moscow, 1951 [English translation U. S. AEC Report AEC-tr-5575 (1963); German translation published by Akademie Verlag].

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Nuclear spin-lattice relaxation in semiquantum liquids

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We calculate in this paper the temperature-dependence of the nuclear spin-lattice relaxation time T_1 of semiquantum liquid hydrogen. We show that T_1 is inversely proportional to the temperature T. Such a T-dependence of T_1 is a universal consequence of the specific properties of semiquantum liquids. The results are in good agreement with experimental data on T_1 measurements in liquid hydrogen.

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Andreev[1-3] has recently developed a theory of semi-quantum liquids. These are liquids in the temperature range $T_d \ll T \ll \Theta$ (Θ is the Debye temperature and T_d determines the quantum indeterminacy of the energy which is connected with the delocalization of the particles in the liquid which is caused by tunnel transitions). In his papers he showed that semi-quantum liquids are characterized by a universal temperature-dependence of the thermodynamic quantities and the kinetic coefficients, which is caused by the specific properties of semi-quantum liquids. He showed, in particular, that the specific heat and the heat conductivity coefficient are proportional to the temperature T while the viscosity is inversely proportional to T, in good agreement with experimental data.

One must expect that the specific properties of semi-quantum liquids will also appreciably alter the temperature-dependence of the spin-lattice relaxation (SLR) time of the nuclei. Indeed, for liquid hydrogen in the temperature range 14 to 20 K one observes experimentally an inverse temperature-dependence of the SLR time of the nuclei[4] and this cannot be explained on the basis of the theory of classical liquids. In this temperature range the hydrogen must have the properties of a semi-quantum liquid.

The aim of the present paper is the calculation of the nuclear SLR time of semi-quantum liquids using the theories developed in the above-mentioned papers.[1-3] When evaluating the SLR time we use a model analogous to the one used by Andreev[3] when calculating the heat conductivity coefficient. For the sake of simplicity we shall assume that the particles have spin $\frac{1}{2}$ (if the particle spin is larger than $\frac{1}{2}$, it will not lead to any alteration in principle of the arguments which follows below) and, by analogy with Ref. 3 that perturbation of the form

$$\hat{V}=-fq,$$

is applied to the system, where q is the operator of the flux of the Zeeman energy between excited states of the particles in the liquid with energies $\varepsilon_1 \pm \hbar\omega_0$ and $\varepsilon_2 \pm \hbar\omega_0$, where ω_0 is the NMR frequency and f is a harmonic generalized force. To evaluate the current q we write down the Hamiltonian of the system:

$$H=H_1+H_2+H_{int},$$

$$H_1=\sum_\sigma \varepsilon_{1\sigma}a_{1\sigma}{}^+a_{1\sigma},\qquad H_2=\sum_\sigma \varepsilon_{2\sigma}a_{2\sigma}{}^+a_{2\sigma},\tag{1}$$

$$H_{int}=J(a_{1+}{}^+a_{2-}+a_{1-}{}^+a_{2+}+a_{2+}{}^+a_{1-}+a_{2-}{}^+a_{1+}),\quad \varepsilon_{i\pm}=\varepsilon_i\pm\hbar\omega_0.\tag{2}$$

J is the interaction constant, and $a_{i\sigma}^-$ and $a_{i\sigma}$ are the creation and annihilation operators for particles in states with energies $\varepsilon_{i\sigma}$. In contrast to Ref. 3 we retain only the interaction which causes the transition of particles between the levels $\varepsilon_{1\pm} - \varepsilon_{2\mp}$, i.e., the transition between the states is accompanied by a spin flip. As we are merely interested in the temperature dependence of the SLR time, we shall not define concretely the interaction mechanism.

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