Electric field on nucleus due to phonon lattice oscillations in solid states

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In atoms and molecules, the electrons screen the nucleus from the external electric field. However, if the frequency of the electric field reaches the energy of atomic or molecular transition, the electric field at the nucleus may be resonantly enhanced by many orders in magnitude. In this paper, we study the mechanisms of screening or enhancement of electric field acting on the nuclei in solid states. We show that in dielectric crystals the phonon oscillations of the lattice play crucial role for determining the electric field on nuclei in the MHz-THz region. As an application, we propose an experimental scheme for measuring nuclear electric dipole moment in a solid state based on the coherent excitation of acoustic phonons.

I. INTRODUCTION

According to Schiff’s theorem [1], atomic electrons screen the nucleus from the external electric field. In particular, a static electric field is completely screened inside neutral atoms and molecules that creates complications in the measurements of nuclear electric dipole moments (EDMs). However, in real atoms and molecules this screening is incomplete due to the magnetic moment effect [1] [2]. Moreover, atomic EDM can be generated by the nuclear Schiff moment and magnetic quadrupole moment [3] [4].

In ions and charged molecules the Schiff screening is incomplete [5] [6], but charged particles accelerate in the electric field and quickly escape. Therefore, EDM measurement experiments with ions require special configurations of the electric and magnetic fields which trap the charged particles [8].

Another interesting possibility to circumvent the Schiff’s screening is to apply oscillating electric field. As is demonstrated in the recent paper [9], the oscillating electric field inside atoms is screened only partly, and the suppression factor is proportional to the dynamic atomic polarizability. From the physical point of view, we understand this result as a lag in the displacement of the electron cloud in the changing electric field. However, when the frequency of the electric field reaches one of the energy levels of atomic transitions, the electric field at nucleus may be enhanced by many orders in magnitude [10].

In molecules, the pattern of screening or resonant enhancement of the oscillating electric field is much richer owing to the presence of rotational and vibrational states in addition to the electronic states [11]. Since the energies of ro-vibrational states are lower than the ones for electronic states, even the fields in the microwave region may strongly interact with nuclei.

This paper is devoted to the extension of our previous results for atoms [9] [10] and molecules [11] to the case of solid states. On the one hand, a crystal can be viewed as a molecule composed of a large number of atoms, and the general consideration developed in Ref. [11] is applicable. However, the general formulae in Ref. [11] do not allow us to give specific numerical estimates as one needs to know exact wavefunctions which take into account positions of all atoms in the solid state including all excitations. On the other hand, in dielectrics and semiconductors, the electric field inside the solid state is well understood through the electric permittivity \( \varepsilon = (1 + \chi)\varepsilon_0 \), where \( \chi \) is the electric susceptibility and \( \varepsilon_0 \) is the vacuum permittivity. Indeed, the electric field \( E \) creates the polarization in the medium \( P = \varepsilon_0 \chi E \) which reduces the electric field in the solid by the factor of \( \varepsilon_r = 1 + \chi \). However, this electric field is macroscopic while we need to know the microscopic electric field acting on each nucleus in the solid state.

In this paper, we consider solid states which are represented by dielectric crystals with no free electrons since the free electrons in metals are responsible for strong screening which is unwanted in our case. As we will demonstrate, it is possible to estimate the electric field at each nucleus when the phonon excitation of the lattice is known. For our estimates, it will be sufficient to consider phonon lattice oscillations semiclassically. Moreover, we will restrict ourselves to the case of harmonic crystal assuming that anharmonic corrections are subleading.

To sketch the main idea, consider a crystal in a state with no phonons such that the atoms in the lattice do not vibrate. This means that each nucleus sits in the minimum of the electrostatic potential of the lattice such that the electric field at the points of the nuclei is vanishing. Assume now that a phonon is excited with a given wavevector \( q \) and frequency \( \omega \). Then, for small perturbations, each atom (or ion) in the lattice oscillates around its equilibrium position harmonically, \( u(t) = u_0 \cos \omega t \), where \( u \) is the deviation of the given atom from its equilibrium position. Discarding the magnetic interaction, one can immediately deduce that each nucleus with mass \( m \) and charge \( Ze \) accelerates in the electric field \( E_{\text{nucl}} = \frac{mE}{Ze} \). Of course, at low temperature, this electric field is very small as the amplitudes of oscillations of atoms in the lattice are tiny. However, the magnitude of this field becomes significant when the lattice vibration is represented by a large number of phonons, e.g., near
the melting temperature of the crystal.\(^1\)

At high temperature, the lattice contains large num-
ber of phonons of all allowed frequencies and wavevectors. In this case, the oscillation of each atom in the lattice is chaotic, with no preferred direction. However, modern technology allows one to coherently create a given num-
er of phonons in the solid state with fixed polarization and frequency, see, e.g., [12, 13]. Thus, when the pattern
of the phonons in the solid state is known, one can de-
duce the value of the oscillating electric field acting on
each nucleus. This technique may be useful in the exper-
iments aiming to study properties of atomic nuclei and,
in particular, the nuclear EDM.

In this paper, unless other units are explicitly specified,
we use natural units, in which \(\hbar = c = 1\), where \(c\) is the
speed of light.

The rest of the paper is organized as follows. In
the next section we derive analytical expressions for the
electric field at nucleus induced by acoustic and optical
phonons in solids. In section III we estimate numerically
the largest magnitude of the electric field of the crystal in
solid xenon created by coherent acoustic phonons. We
also consider the optical phonons in a sodium chlorine
crystal and show that they may enhance the external
electric field acting on the nucleus when the frequency of
this field is in resonance with the frequency of transverse
optical phonons. In section IV, we present a novel theo-
retical idea how the coherently excited acoustic phonons
may be used in experiments aimed at measuring the per-
manent nuclear EDM. In the last section we summarize
and briefly discuss the obtained results.

II. THEORY

In this section, we derive analytical expressions for the
value of the electric field acting on nuclei in crystals due
to acoustic and optical phonons. In our derivation we re-
strict ourselves to the theory of harmonic crystals leaving
the analysis of anharmonic corrections for further stud-
ies.

A. Electric field due to acoustic phonons

Acoustic phonons with long wavelengths may be con-
sidered as sound waves in a continuous medium with a
frequency \(\omega\) and a wave vector \(q\),

\[
u(r, t) = u_0 \cos(q \cdot r - \omega t),
\]

where \(u_0\) is the amplitude. Consider, in particular, the
oscillations of the atom at \(r = 0\), in the direction \(u_0 =
(0, 0, u_0)\), \(u(t) = u_0 \cos \omega t\). This oscillation reaches
the maximum amplitude when the crystal is nearly melted
or destroyed. Typically, this oscillation amplitude is of
order \(0.1\) of interatomic distance \(a\),

\[u_{0, \text{max}} \approx 0.1a.\]

Thus, in the harmonic approximation, we know the os-
cillation pattern of the atomic nucleus,

\[u(t) = 0.1a \cos \omega t.\]

This motion is produced by the microscopic electric field
acting on nucleus,

\[E_{\text{nucl}} = \frac{m}{Ze} \ddot{u} = -\frac{0.1 a m \omega^2}{Ze} \cos \omega t,\]

where \(m\) is the mass of the nucleus and \(Ze\) is its charge.
Thus, the maximum amplitude of the electric field on
nucleus due to acoustic phonons reads

\[E_0 = -\frac{0.1 a m \omega^2}{Ze}.\]

As we will show in section III A, for low frequencies this
electric field may be much stronger than the screened
external electric field.

B. Electric field due to optical phonons

Let us consider a simple cubic lattice with two ions
per unit cell. Let \((u_1, m_1)\) and \((u_2, m_2)\) be pairs of co-
ordinates and masses of the two ions in the unit cell. To
describe the oscillations around the common center of
mass, it is convenient to introduce the phonon coordi-
nate

\[u = \sqrt{mN}(u_1 - u_2),\]

where \(m\) is the reduced mass, \(m^{-1} = m_1^{-1} + m_2^{-1}\), and \(N\)
is the atom number density. In the external oscillating
electric field \(E = E_0 \cos \omega t\) the dynamics of the variable
\(u\) is described by the equation

\[\ddot{u} + \gamma \dot{u} + \omega^2 u = Z^* E_0 \cos \omega t,\]

where \(\gamma\) is the phonon inverse lifetime, \(\omega_i\) is the trans-
verse optical phonon frequency and \(Z^*\) is the effective
ion charge. The latter may be expressed via the dielec-
tric constants of the solid state (see, e.g., [14]),

\[Z^* = \omega_i \sqrt{\frac{\varepsilon_{\text{stat}} - \varepsilon_{\text{opt}}}{4\pi \varepsilon_{\text{opt}}} \frac{3}{\varepsilon_{\text{opt}} + 2}},\]

where \(\varepsilon_{\text{stat}}\) and \(\varepsilon_{\text{opt}}\) are the electric permittivity for static and high-frequency electric fields, respectively.

In the harmonic approximation, both \(\omega_i\) and \(Z^*\) are constants. More generally, one can consider the phonon

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\(^1\) In liquids, longitudinal sound waves also produce the electric field at nuclei. However, in this paper we focus on solids only.
dynamics with anharmonic corrections, but this problem is beyond the scope of this paper.

The steady state solution of the equation \( \ddot{u} = \dot{u}_0 \cos(\omega t + \phi) \), \( \phi = \arctan \left( \frac{\omega \gamma}{\omega^2 - \omega_1^2} \right) \), \( \omega_1 = \frac{\sqrt{q^2 \omega^2 - (\omega_0)^2}}{} \), \( \omega_0 = \frac{Z^* E_0}{\sqrt{\omega_1^2 - 2 \omega_1^2 + (\omega \gamma)^2}} \), \( E_{\text{ion}} = \frac{1}{q} \sqrt{\frac{m}{N}} u_0 = -\frac{\omega^2}{q} \sqrt{\frac{m}{N}} u_0 \cos(\omega t + \phi) \), \( E_{\text{ion,0}} = -\frac{\omega^2}{q} \sqrt{\frac{m}{N}} u_0 \), \( E_{\text{ion,0}} = \frac{Z^*}{q} \sqrt{\frac{m}{N}} \frac{\omega^2}{\omega_1^2 - \omega^2} E_0 \) reads

The electric field acting on the ions can be found as

\[
E_{\text{ion}} = \frac{1}{q} \sqrt{\frac{m}{N}} u_0 = -\frac{\omega^2}{q} \sqrt{\frac{m}{N}} u_0 \cos(\omega t + \phi),
\]

where \( q \) is the charge of the ion. The amplitude of this field is

\[
E_{\text{ion},0} = -\frac{\omega^2}{q} \sqrt{\frac{m}{N}} u_0 \approx \frac{Z^*}{q} \sqrt{\frac{m}{N}} \frac{\omega^2}{\omega_1^2 - \omega^2} E_0.
\]

When the frequency of the external electric field \( \omega \) is far from the phonon resonance frequency \( \omega_1 \), \( \omega \ll \omega_1 \), the equation \( \ddot{u} = \dot{u}_0 \cos(\omega t + \phi) \) reduces to

\[
E_{\text{ion},0} = \frac{Z^*}{q} \sqrt{\frac{m}{N}} \frac{\omega^2}{\omega_1^2 - \omega^2} E_0.
\]

On the contrary, near resonance, \( \omega \approx \omega_1 \), \( |\omega - \omega_1| \ll \gamma \), the amplitude of the electric field amplitudes,

\[
E_{\text{ion,0}} = \frac{Z^*}{q} \sqrt{\frac{m}{N}} \omega_1 E_0.
\]

Finally, we point out that the bound electrons of each ion further screen the electric field on the nucleus by the law \( \ddot{u} = \dot{u}_0 \cos(\omega t + \phi) \), \( \phi = \arctan \left( \frac{\omega \gamma}{\omega^2 - \omega_1^2} \right) \), \( \omega_1 = \frac{\sqrt{q^2 \omega^2 - (\omega_0)^2}}{} \), \( \omega_0 = \frac{Z^* E_0}{\sqrt{\omega_1^2 - 2 \omega_1^2 + (\omega \gamma)^2}} \), \( E_{\text{nucl}} = E_{\text{ion}} \left( 1 - \frac{N_e}{Z} - \alpha_{\text{ion}}(\omega) \frac{\omega^2 m_e^2}{Z e^2} \right), \)

where \( N_e \) is the number of electrons in the ion, \( Z \) is the charge of the nucleus and \( \alpha_{\text{ion}}(\omega) \) is the atomic polarizability of the ion.

### III. NUMERICAL ESTIMATES

In this section, we give numerical estimates of the electric field on nucleus induced by acoustic and optical phonons. For the acoustic phonons, we consider solid xenon because it may be further applied in nuclear EDM measurement experiments. The electric field due to the optical phonons is considered in the sodium chlorine crystal because its optical and dielectric properties are well represented in the literature.

#### A. Electric field in solid xenon

Let us consider \(^{129}\text{Xe}\) noble gas in the solid state below the melting temperature \( T_{\text{melt}} = 161 \text{ K} \). The nuclear magnetic dipole moment of this isotope is \( \mu \approx -0.78 \mu_N \) \[^{13}\] \( \mu_N \) is the nuclear magneton. In a strong magnetic field \( B = 10 \text{ T} \), the nuclear spin Larmor precession frequency is \( \omega = 2\mu_B B = 119 \text{ MHz} = 4.9 \times 10^{-7} \text{ eV} \). We will be interested in acoustic phonons in the xenon crystal with this frequency \( \omega \).

The crucial assumption in our estimate will be that it is possible to coherently excite the phonons in the solid state with the given frequency and the wave vector. In particular, it is possible to use a pulsed laser with pulses modulated to a given frequency \( \omega \) to coherently generate acoustic phonons, see, e.g. \[^{12}\] \( \omega_t \) for a review. Moreover, we point out that the modern technology allows one to measure precisely the number of phonons created in the solid state \[^{15}\] \( \omega_0 \). Without going further into the details of these techniques we will assume that they may be applied to a solid xenon sample.

Given that the lattice parameter in the solid xenon is \( a = 6.2 \text{ Å} \), the maximum electric field at the nucleus may be estimated from Eq. (5):

\[
E_{\text{nucl}} = 0.9 \text{ V/m}.
\]

It is instructive to compare the electric field due to phonon lattice vibrations with the screening of the external electric field on the nucleus in an isolated Xe atom. According to \[^{9}\], the electric field at the nucleus induced by the external electric field \( E = E_0 \cos(\omega t) \) is

\[
E_{\nucl} = \frac{\tilde{\alpha} \omega^2}{Z} E \approx 1.6 \times 10^{-16} E,
\]

where \( \tilde{\alpha} = 27.3 \) is the static atomic polarizability of xenon and \( \tilde{\omega} = \omega B/\epsilon_0 = 1.8 \times 10^{-8} \) is the energy in atomic units. Thus, for any reasonable laboratory electric field \( E_0 \) the electric field on the nucleus due to phonons \( \omega \) is much stronger than the external electric field screened by the atomic electrons \( \omega_0 \).

#### B. Electric field due to optical phonons in sodium chloride

Dielectric and phonon properties of NaCl are well known, see, e.g. \[^{13}\]. In particular, the electric permittivity for the static and optical frequency electric fields is \( \varepsilon_{\text{stat}} = 5.9 \), \( \varepsilon_{\text{opt}} = 2.34 \), and the transverse optical phonon resonant frequency is \( \omega_t = 0.02 \text{ eV} \). The phonon width \( \gamma \) may be estimated as \( \omega_t/\gamma \approx 50 \) \[^{16}\]. The reduced mass for the NaCl molecule is \( m = 13.9 m_p \), and the atom number density is \( N \approx 2 \times 10^{22} \text{ cm}^{-3} \). According to Eq. (15), the electric field acting on each ion is

\[
E_{\text{ion},0} = 39 E_0.
\]
Given the electric field at ion, the field at nucleus may be obtained with Eq. (16). At the frequency \( \omega = \omega_L \) the last term in Eq. (16) is negligible. Then, for the Na ion \( Z = 11 \) and \( N_e = 10 \), and we have

\[
E_{\text{nucl}} \approx \frac{1}{\mu} E_{\text{ion}} \approx 3.5 E.
\]  

(20)

Thus, the oscillating electric field in resonance with the transverse optical phonons not only reaches the nucleus, but may also be enhanced by the factor of 3.5.

Note that, in Eq. (20), the electric field at the nucleus grows linearly with \( E \) only for a weak external field when the harmonic description of phonons applies. We stress that the magnitude of the electric field cannot exceed the value (5) at which the lattice oscillations reach the maximum amplitude. For the \( \text{NaCl} \) crystal, this maximum electric field is of order \( 10^7 \) V/m at the frequency \( \omega = \omega_L = 480 \text{ GHz} \).

Note also that if one considers the electric field off the resonance with the optical phonon frequency, the equation (14) applies. In this case, instead of the resonance enhancement there is off-resonance suppression.

IV. APPLICATION: NUCLEAR EDM MEASUREMENT

Recently, there have been proposed a few experiments to measure nuclear or electron EDMs with solid state samples \[17-21\]. It is expected that such experiments may have a better sensitivity as compared to the traditional EDM experiments on atoms and molecules in vapor state or in beams. However, as was noticed in \[19,22\], one of the issues of the solid-state EDM experiments is that the oscillating strong electric field causes the heating of the sample and thermal depolarization of spins. However, this problem does not arise in the CASPEr experiment \[22,23\] aimed at the detection of oscillating EDM induced by axion dark matter.

In this section, we will present a novel idea how to measure permanent nuclear EDM using the phonon excitations in solids. We will consider an experimental setup similar to the CASPEr experiment \[22,23\], but with important modifications needed to measure permanent nuclear EDM. A very schematic design of this experiment with main emphasis on the orientation of electric and magnetic fields is shown in Fig. 1. Nuclear spins in this solid state are pre-polarized by the external strong magnetic fields. The orientation of magnetic and electric fields in the solid-state EDM experiments is shown in Fig. 1. Nuclear spins in this solid state are pre-polarized by the external strong magnetic fields is created by a strong magnet while the electric field \( E \) is the microscopic electric field on nuclei created by coherent phonon lattice oscillations in the given direction. The interaction of nuclear EDM with oscillating electric field creates the transverse macroscopic magnetization \( M \) of the sample which may by detected by a SQUID magnetometer.

The above estimate is very close to current experimental limits on the nuclear EDM. The best limit on the atomic EDM in xenon was obtained in Ref. \[24\]: \(|d_{\text{Xe}}| < 1.5 \times 10^{-27} \text{ e} \cdot \text{cm} \). According to Ref. \[2\], in
xenon, the nuclear EDM contributes to the atomic EDM as $d_{xe} = 4.4 \times 10^{-6} d_N$. Thus, the xenon EDM experiment puts the following limit on the nuclear EDM in xenon:

$$|d_N| < 2.5 \times 10^{-22} \text{ e cm.} \quad (23)$$

As a result, it is may be promising to develop an experimental technique for measuring nuclear EDM using the phonon lattice oscillations.

We stress that Eq. (22) represents a very crude estimate of sensitivity of an experiment aimed at measuring the nuclear EDM in solids using lattice oscillations. In a more accurate estimate one is to analyse the signal to noise ratio by taking into account different noise sources in realistic experiments. This analysis will be done elsewhere. Here we only present the theoretical idea of possible application of coherent phonon excitations in solids to the nuclear EDM measurement. We point out that our proposal is novel as it allows for direct nuclear EDM measurement which is free from the problem of Schiff’s screening.

Finally, we point out that the experimental technique described in this section may be applied to ionic crystals. In this case, it might be possible to measure the EDMs of ions induced by the nuclear Schiff moment, magnetic quadrupole moment or electron EDM.

V. SUMMARY

In this paper, we estimated the magnitude of the electric field induced on the atomic nuclei by phonon lattice oscillations in solid states. In these oscillations, the maximum deviation of atoms from their equilibrium positions is typically of order of one tenth of the interatomic distance that corresponds to the maximum magnitude of the electric field acting on the nuclei as in Eq. (5). If the atoms oscillate randomly due to the thermal motion, this field averages out in time. However, if the acoustic phonons can be created coherently in all atoms in the solid state with a given wave vector and polarization, this electric field becomes significant. As we demonstrated, for low frequencies (characteristic to the acoustic phonons) this electric field acting on atomic nuclei due to phonon lattice oscillation is much stronger than the external electric field screened by the atomic electrons. In particular, in solid xenon, this field is of order 1 V/m at the frequency 119 MHz.

The crucial assumption in our estimate is that the acoustic phonons may be excited coherently with given wave vector and polarization. This assumption is based on the advances in the phonon generation and counting, see, e.g., [12, 13]. As we advocate in section IV, this technique may be applied to measure the nuclear EDM. We expect that possible NMR-like experiments based on the phonon lattice oscillations may be sensitive to the nuclear EDM of order $10^{-22}$ e·cm. This sensitivity is very close to the current constraint on the nuclear EDM (23) arising from the recent atomic EDM measurement in xenon [23]. Thus, it is tempting to develop the experimental technique for measuring the nuclear EDM with phonon lattice oscillations in solids.

We also estimated the electric field at nucleus due to optical phonons which are present in many ionic crystals. In contrast to the acoustic phonons, the optical ones interact directly with the external electric field. When this electric field is in resonance with the frequency of transverse optical phonons, it may be enhanced on the nucleus. Possible experimental applications of the electric field at nucleus induced by the optical phonons will be discussed elsewhere.

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