

# Optical cavity tests of Lorentz invariance for the electron

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A hypothetical violation of Lorentz invariance in the electrons' equation of motion (expressed within the Lorentz-violating extension of the standard model) leads to a change of the geometry of crystals and thus shifts the resonance frequency of an electromagnetic cavity. This allows experimental tests of Lorentz invariance of the electron sector of the standard model. The material dependence of the effect allows to separate it from an additional shift caused by Lorentz violation in electrodynamics, and to place independent limits on both effects. From present experiments, upper limits on Lorentz violation in the electrons' kinetic energy term are deduced.

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## I. INTRODUCTION

Special relativity and the principle of Lorentz invariance describe how the concepts of space and time have to be applied when describing physical phenomena in flat space–time. Improving the accuracy of the experimental verification of these fundamental concepts is of great interest, also because a violation of Lorentz invariance is a feature of many current models for a quantum theory of gravity, e.g., string theory [1, 2], loop gravity [3, 4], and non-commutative geometry [5]. Such a violation of Lorentz invariance is described in the general standard model extension (SME) developed by Colladay and Kostelecký [6]. According to it, Lorentz violating terms might enter the equations of motion of bosons and fermions. At first sight, the quantum gravity induced corrections and effects are of order  $E/E_{\text{QG}} \sim 10^{-28}$  where  $E$  is the energy scale of the experiment (which in ordinary optical experiments is of the order 1 eV) and  $E_{\text{QG}} \sim E_{\text{Planck}}$  is of the order of the Planck energy. Therefore these effects seem to be far from being observable in laboratory experiments. However, as it occurs e.g. in scenarios leading to a modification of the Newton potential at small distances, some mechanism may apply which effectively leads to much larger effects in the laboratory. It is thus interesting to find experimental configurations in the laboratory that can place strong upper limits on as many of these terms as possible.

Experiments on Lorentz symmetry that study light propagation have a long and fascinating history, starting from the original interferometer experiments of Michelson [7] in Potsdam and Michelson and Morley [8] in Cleveland. Modern versions of these experiments [9, 10, 11, 12, 13, 14, 15] replace the interferometer by a mea-

surement of the resonance frequency  $\nu = mc/(2L)$  of an electromagnetic (Fabry-Pérot) cavity, that is given by the velocity of light  $c$  along the cavity axis, the cavity length  $L$ , and a constant mode number  $m$ . Lorentz violation causing a shift of  $c$  or  $L$  connected to a rotation or boost of the cavity frame of reference can thus be detected through the corresponding shift of the resonance frequency. From such experiments, upper limits on a tensor  $(k_F)_{\kappa\lambda\mu\nu}$  have been found, that encodes Lorentz violation in the photonic sector of the SME [12, 13, 15, 16, 17, 18]. These experiments are mainly based on the shift of  $c$  connected to non-zero values of  $(k_F)_{\kappa\lambda\mu\nu}$ , as an additional change of  $L$  caused by  $(k_F)_{\kappa\lambda\mu\nu}$  and a corresponding orientation dependent modification of the Coulomb potential is negligible for most cavity materials [19].

In this work, we treat the effect of Lorentz violation within the fermionic sector of the standard model extension in cavity experiments. A modified kinetic energy term entering the non-relativistic Schrödinger hamiltonian of the free electron  $(p^2 + 2E'_{jk}p_jp_k)/(2m)$  leads to a change of the geometry of crystals, and thus a change  $\delta_{e-\nu}$  of the resonance frequency of a cavity made from this crystal. Here,  $p_j$  is the 3-momentum,  $m$  the electron mass, and  $E'_{jk} = -c_{jk} - c_{00}\delta_{jk}$  a dimensionless  $3 \times 3$  matrix given by a tensor  $c_{\mu\nu}$  of the SME. Thus, the total shift of the resonance frequency  $\delta\nu = \delta_{e-\nu_{res}} + \delta_{\text{EM}}\nu_{res}$ , where  $\delta_{\text{EM}}\nu$  denotes the shift due to Lorentz violation in the electromagnetic sector. Since  $\delta_{e-\nu}$  depends on the cavity material, it can be distinguished from Lorentz violation in electrodynamics by comparing cavities made from different materials. Experiments using suitable configurations of cavities can place separate upper limits on the components of  $c_{\mu\nu}$  and  $(k_F)_{\kappa\lambda\mu\nu}$ . Using data available from past experiments, we deduce approximate bounds on some combinations of components of  $c_{\mu\nu}$  at the  $10^{-14}$  level. From future cavity experiments, Earth and space-based, that are projected as tests of Lorentz violation in electrodynamics [20, 21, 22], bounds at a level down to  $10^{-18}$  can be expected.

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In Sec. II, we present the non-relativistic hamiltonian of the free electron within the SME. Since violations of Lorentz invariance are certainly small, it is sufficient to work to first order in the Lorentz-violating modifications throughout. The crystal adjusts its geometry such as to minimize the total energy  $\langle \delta h \rangle + U_{\text{elast}}$ , where  $\langle \delta h \rangle$  is the expectation value of the Lorentz-violating part of the hamiltonian and  $U_{\text{elast}}$  is the elastic energy associated with distortion of the crystal. It is calculated in Sec. III. The resulting geometry change is calculated in Sec. IV. A fairly detailed model for the crystal allows us to obtain specific results for practical materials, including quartz and sapphire. In Sec. V, we discuss experimental configurations and obtain bounds on Lorentz violation in the electrons' equation of motion from present experiments. In appendix A, we discuss the hypothetical case of a cavity made from a spin-polarized solid, which allows to place experimental limits on an additional, spin dependent term from the SME, at least in principle. In appendix B, we summarize some conventions made in elasticity theory that are needed for our calculations, and in appendix C, we give in detail the Fourier components of the signal for Lorentz violation in laboratory experiments on Earth.

## II. STANDARD MODEL EXTENSION

### A. Model

The SME starts from a Lagrangian formulation of the standard model, adding all possible observer Lorentz scalars that can be formed from the known particles and Lorentz tensors. Taken from the full SME that contains all known particles, the Lagrangian involving the Dirac fields  $\psi^e$  of the electron and  $\psi^p$  of the proton and the electromagnetic field  $F^{\mu\nu}$  can be written as (in this section, we use units with  $\hbar = c = 1$ ; the greek indices take the values 0, 1, 2, 3) [6, 23]

$$\begin{aligned} \mathcal{L} = & \frac{i}{2} \bar{\psi}^e \Gamma_\nu^e D^\nu \psi^e - \frac{1}{2} \bar{\psi}^e M^e \psi^e + \frac{i}{2} \bar{\psi}^p \Gamma_\nu^p D^\nu \psi^p \\ & - \frac{1}{2} \bar{\psi}^p M^p \psi^p + \text{h.c.} - \frac{1}{4} F^{\mu\nu} F_{\mu\nu} \\ & - \frac{1}{4} (k_F)_{\kappa\lambda\mu\nu} F^{\kappa\lambda} F^{\mu\nu} + \frac{1}{2} (k_{AF})^\kappa \epsilon_{\kappa\lambda\mu\nu} A^\lambda F^{\mu\nu}, \end{aligned} \quad (1)$$

where h.c. denotes the hermitian conjugate of the previous terms, and  $A^\lambda$  is the vector potential. The symbols  $\Gamma_\nu^{e,p}$  and  $M^{e,p}$  are given by

$$\begin{aligned} \Gamma_\nu &= \gamma_\nu + c_{\mu\nu} \gamma^\mu + d_{\mu\nu} \gamma_5 \gamma^\mu + e_\nu + i f_\nu \gamma_5 + \frac{1}{2} g_{\lambda\mu\nu} \sigma^{\lambda\mu}, \\ M &= m + a_\mu \gamma^\mu + b_\mu \gamma_5 \gamma^\mu + \frac{1}{2} H_{\mu\nu} \sigma^{\mu\nu}, \end{aligned} \quad (2)$$

where the superscripts  $e$  and  $p$  are to be added to the symbols  $a_\mu, b_\mu, c_{\mu\nu}, d_{\mu\nu}, e_\mu, f_\mu, g_{\lambda\mu\nu}$ , and  $H_{\mu\nu}$  that represent tensors encoding Lorentz violation for the fermions.

$m^e$  and  $m^p$  are the electron and the proton mass,  $\gamma_\nu, \gamma_5$  and  $\sigma^{\mu\nu}$  are the conventional Dirac matrices, and  $D^\nu$  is the covariant derivative. In this work, we deal mostly with electrons and add a superscript to denote parameters for particles other than the electron, e.g.,  $c_{\mu\nu}$  is a parameter for the electron and  $c_{\mu\nu}^p$  the corresponding parameter for the proton. The tensors entering  $M$  have the dimension mass, the others are dimensionless.  $H_{\mu\nu}$  is antisymmetric;  $g_{\lambda\mu\nu}$  is antisymmetric in its first two indices.  $c_{\mu\nu}$  and  $d_{\mu\nu}$  are traceless. Gauge invariance and renormalizability excludes  $e_\nu, f_\nu$ , and  $g_{\lambda\mu\nu}$ , so these are either zero or suppressed relative to the others [23].

Lorentz violation for the photons is encoded in the tensors  $(k_{AF})^\kappa$  and  $(k_F)_{\kappa\lambda\mu\nu}$ . The four degrees of freedom contained in  $(k_{AF})^\kappa$  are constrained strongly in measurements of cosmological birefringence [17, 18] and are neglected in what follows. 10 of the 19 degrees of freedom of  $(k_F)_{\kappa\lambda\mu\nu}$  are constrained by astrophysical observations [17, 18], the other 9 can be measured in cavity experiments [13, 15, 16, 17, 18].

### B. Modified non-relativistic hamiltonian

#### 1. Free electron

The non-relativistic Schrödinger hamiltonian  $h = \hat{h} + \delta h$  of a single free electron within the SME derived from this Lagrangian (using Foldy-Wouthuysen methods, [24]) is the sum of the usual free-particle Hamiltonian  $\hat{h}$  and a Lorentz-violating term [23, 24]

$$\begin{aligned} \delta h = & m A' + m B'_j \sigma^j + C'_j p_j + D'_{jk} p_j \sigma^k \\ & + E'_{jk} \frac{p_j p_k}{m} + F'_{jkl} \frac{p_j p_k}{m} \sigma^l \end{aligned} \quad (3)$$

with the components of the 3-momentum  $p_j$  and of the Pauli matrices  $\sigma^j$ . The latin indices take the values 1, 2, 3. (We denote both 3-vectors such as  $x_j$  and reciprocal 3-vectors such as  $p_j$  by subscript.) A Hamiltonian of this form has also been derived in [25]. The constant term  $m A'$  has no physical consequences and is included for completeness. The term proportional to  $C'_j$  can be eliminated by choosing coordinates such that the systems centre of mass is at rest [25]. The dimensionless coefficients  $A', B'_j, C'_j, D'_{jk}, E'_{jk}$  and  $F'_{jkl}$  can be expressed in terms of the quantities entering the Lagrangian [23, 24]:

$$A' = \frac{1}{m} a_0 - c_{00} - e_0, \quad (4)$$

$$B'_j = -\frac{b_j}{m} + d_{j0} - \frac{1}{2} \varepsilon_{jkl} g_{kl0} + \frac{1}{2m} \varepsilon_{jkl} H_{kl}, \quad (5)$$

$$C'_j = -\frac{a_j}{m} + (c_{0j} + c_{j0}) + e_j, \quad (6)$$

$$\begin{aligned} D'_{jk} = & \frac{b_0}{m} \delta_{jk} - (d_{kj} + d_{00} \delta_{jk}) \\ & - \varepsilon_{klm} \left( \frac{1}{2} g_{mlj} + g_{m00} \delta_{jl} \right) - \frac{1}{m} \varepsilon_{jkl} H_{l0}, \end{aligned} \quad (7)$$

$$E'_{jk} = -c_{jk} - \frac{1}{2}c_{00}\delta_{jk}, \quad (8)$$

$$F'_{jkl} = \left[ (d_{0j} + d_{j0}) - \frac{1}{2} \left( \frac{b_j}{m} + d_{j0} + \frac{1}{2}\varepsilon_{jmn}g_{mn0} + \frac{1}{2m}\varepsilon_{jmn}H_{mn} \right) \right] \delta_{kl} + \frac{1}{2} \left( \frac{b_l}{m} + \frac{1}{2}\varepsilon_{lmn}g_{mn0} \right) \delta_{jk} - \varepsilon_{jlm}(g_{m0k} + g_{mk0}). \quad (9)$$

## 2. Interaction terms

In addition to  $\delta h$ , the Hamiltonian arising from the Lagrangian Eq. (1) also involves modified interaction terms proportional to combinations of  $a_\mu, b_\mu, c_{\mu\nu}, d_{\mu\nu}, e_\mu, f_\mu, g_{\lambda\mu\nu}$ , and  $H_{\mu\nu}$ . For the non-relativistic electrons in solids, however, these are suppressed by a factor given by  $\alpha$ , the fine-structure constant, relative to the modifications of the free-particle Hamiltonian, Eq. (3) [23]. This is basically because the typical energy scale for such electrons is the Rydberg energy  $m\alpha^2/2$ . We can therefore neglect the modified interaction terms.

## C. Coordinate and field redefinitions

Some of the parameters contained in either the photon, electron, or proton sectors of the Lagrangian Eq. (1) can be absorbed into the other sectors by coordinate and field redefinitions without loss of generality. Thus, not all of the coefficients in the Lagrangian have separate physical meanings. Loosely speaking, in experiments where one compares the sectors against each other only differential effects are meaningful.

For example, in a hypothetical world containing only photons and electrons, the nine components of  $(k_F)_{\kappa\lambda\mu\nu}$  not constrained by astrophysical experiments could be absorbed into the nine symmetric components of  $c_{\mu\nu}^e$  [6, 17, 18, 26]. By definition, either the photon or the electron sector could be taken as conventional with all the Lorentz violation in the other sector. For example, for tests of Lorentz violation for the photon [13, 15, 16, 17, 18], one implicitly assumes a conventional electron sector.

The presence of protons (and neutrons) in the solid changes this picture. We can still assume that one of the sectors is conventional, but then in general the other sectors are Lorentz-violating. Choosing a conventional proton sector allows us to disregard the proton terms. It also fixes the definition of coordinates and fields so that the components of  $c_{\mu\nu}$  cannot be absorbed into  $(k_F)_{\kappa\lambda\mu\nu}$  in general, i.e. they acquire separate physical meanings.

To illustrate this, it suffices to consider an extension of the toy version of the SME introduced in [18]. Its Lagrangian describes electrons and protons as scalar fields  $\phi^e$  and  $\phi^p$ , neglecting spin effects:

$$\mathcal{L}^\phi = (\eta_{\mu\nu} + k_{\mu\nu})(D_\mu\phi^e)^\dagger D_\nu\phi^e - m^2(\phi^e)^\dagger\phi^e$$

$$+ (D_\mu\phi^p)^\dagger D^\mu\phi^p - (m^p)^2(\phi^p)^\dagger\phi^p - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} - \frac{1}{4}(k_F)_{\kappa\lambda\mu\nu}F^{\kappa\lambda}F^{\mu\nu}. \quad (10)$$

It has a conventional proton sector and non-conventional electron and photon sectors. Lorentz violation for the electron is given by the coefficient  $k_{\mu\nu}$ . As usual, the covariant derivative is given by  $D_\mu\phi^{e,p} = (\partial_\mu + iq^{e,p}A_\mu)\phi^{e,p}$ , where  $q^{e,p}$  is the particle's electric charge. If one identifies  $k_{\mu\nu} = c_{\mu\nu}^e$ , this Lagrangian leads to the modified Hamiltonian Eq. (3) if only the  $c_{\mu\nu}$  are nonzero.

For simplicity, consider the special case of only one nonzero component  $k_{00} = k^2 - 1$ , where  $k$  deviates slightly from unity. The lagrangian takes the form [18]

$$\mathcal{L}^\phi = (D_\mu\phi^e)^\dagger D_\nu\phi^e + (k^2 - 1)|D_0\phi^e|^2 - m_e^2(\phi^e)^\dagger\phi^e + (D_\mu\phi^p)^\dagger D^\mu\phi^p - (m^p)^2(\phi^p)^\dagger\phi^p - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} - \frac{1}{4}(k_F)_{\kappa\lambda\mu\nu}F^{\kappa\lambda}F^{\mu\nu}. \quad (11)$$

By coordinate transformations  $t \rightarrow tk$ ,  $\vec{x} \rightarrow \vec{x}$ , the field redefinition  $A_0 \rightarrow A_0$ ,  $A_i \rightarrow A_i k$ , and rescaling the electric charge  $q \rightarrow q/k$ , one obtains the Lagrangian

$$\mathcal{L}^\phi = (D_\mu\phi^e)^\dagger D_\nu\phi^e - m^2(\phi^e)^\dagger\phi^e + (D_\mu\phi^p)^\dagger D^\mu\phi^p + (k^{-2} - 1)|D_0\phi^p|^2 - (m^p)^2(\phi^p)^\dagger\phi^p - \frac{1}{4}F^{\mu\nu}F_{\mu\nu} - \frac{1}{4}(k_F)_{\kappa\lambda\mu\nu}F^{\kappa\lambda}F^{\mu\nu} + \frac{1 - k^2}{2}B^2,$$

where  $B$  is the magnetic field. Thus, the Lorentz violation in the electron sector has been moved to the proton and photon sectors. (If  $(k_F)_{\kappa\lambda\mu\nu} = 0$ , the parameter  $1/k$  can be interpreted as a modified velocity of light [18].) However, it is in general not possible to eliminate Lorentz violation in more than one sector at the same time.

Cavity experiments compare the velocity of a light wave to a length defined by a crystal. In the light of Eq. (11), the Lorentz violation for the electron acts via the term  $(k^2 - 1)|D_0\phi^e|^2$ . With a time-independent Coulomb potential  $A_0 = \text{const.}$ , this contributes a term

$$- 2im(k^2 - 1)[\phi_{,0} + q\Re(A_0)\phi] \quad (13)$$

to the equation of motion for  $\Phi^e = e^{-imx_0}\phi^e$  in the non-relativistic limit (obtained, in the usual way, by the Euler-Lagrange equations and setting to zero terms of order  $|A_0|^2$  and  $m^0$ ).  $\Re$  denotes the real part. The second term modifies the coupling of the electron to the Coulomb potential, causing a geometry change of the crystal. Thus, a combination of  $k^2 - 1$  and the modified velocity of light given by  $(k_F)_{\kappa\lambda\mu\nu}$  is measured in the experiment.

In the alternative description by Eq. (12), the same Lorentz violation acts via a term analogous to Eq. (13) in the equation for the proton, i.e., a rescaled coupling of the proton to the electric field, and a modified velocity of light given by  $(k_F)_{\kappa\lambda\mu\nu}$  and  $k^2 - 1$ . Physically, both pictures are equivalent.

Here, we considered only a single parameter analogous to  $c_{00}$ , that causes a scaling of the solid that is rotation-invariant. Thus, it cannot be measured in usual cavity experiments, that search for a modulation of the effect connected to a rotation of the cavity in space. However, the tensors  $c_{\mu\nu}$  emerging from our special case via the three Lorentz boosts can — i.e., at least three out of nine degrees of freedom contained in the symmetric part of  $c_{\mu\nu}$ . It is not impossible that, by coordinate and field redefinitions, some of the other parameters can be absorbed into quantities that have no measurable effect. However, as we have shown, at least 12 out of 18 parameters from the photon and electron sector (restricting the electron sector to those parameters that are not constrained by cosmological experiments) would be separately measurable, that can e.g. be chosen as three  $c_{\mu\nu}$  and nine  $(k_F)_{\kappa\lambda\mu\nu}$ .

In what follows, we adopt a conventional proton sector, with all the Lorentz violation in the electron and photon sectors. One could possibly extract the measurable quantities from  $c_{\mu\nu}$  and consider only those in what follows; however, thereby one would single out a preferred frame in which the measurable quantities are defined, and loose the covariance under observer Lorentz transformations which otherwise holds in the SME. Therefore, we choose not to do so and treat all elements of  $c_{\mu\nu}$  as independent.

#### D. Previous experimental limits on electron parameters

It is convenient to express limits on the coefficients within a sun-centered celestial equatorial reference frame as defined in [23]. The components of quantities given in that frame are denoted by capital indices. Limits for many particles, including muons, protons, and neutrons, have been studied, see [22, 23, 27] and references therein. For the electron, the limits given below have been found. However, to our knowledge there are no experimental limits on  $E'_{jk}$  and on many components of  $F'_{jkl}$  for the electron.

From clock comparison experiments [23], a limit on  $B_J \lesssim 10^{-24}$  ( $mB_J$  is denoted  $\tilde{b}_J$  in [23]) is obtained. Furthermore, for the linear combinations

$$\begin{aligned} \tilde{d}_J &= m(d_{0J} + d_{J0}) - \frac{1}{2} \left( md_{J0} + \frac{1}{2} \varepsilon_{JKL} H_{KL} \right), \\ \tilde{g}_{D,J} &= m\varepsilon_{JKL}(g_{K0L} + \frac{1}{2} g_{KLO}) - b_J, \end{aligned} \quad (14)$$

$\tilde{d}_J/m \lesssim 10^{-19}$  and  $\tilde{g}_{D,J}/m \lesssim 10^{-19}$ . These are order-of-magnitude limits, since some assumptions are needed to extract them from the measurements [23].

An experiment using spin polarized solids yielded  $|B'_Z| \simeq (2.7 \pm 1.6) \times 10^{-25}$  [28, 29]; in a similar experiment [30],  $((B'_X)^2 + (B'_Y)^2)^{1/2} \leq 6.0 \times 10^{-26}$  and  $|B'_Z| \leq 1.4 \times 10^{-25}$  have been found.

Hydrogen spectroscopy could prospectively limit linear combinations of  $B'_J, B'_J{}^p, d_{J0}, d^p_{J0}, H_{JK}$ , and  $H^p_{JK}$  (where

the superscripts  $p$  denotes parameters for the proton) to about  $10^{-27}$  GeV [31]. Comparing the frequencies of hydrogen masers, [32] find  $|B'_J{}^p m^p + B'_J m| \lesssim 2 \times 10^{-28}$  GeV ( $m$  and  $m^p$  are the electron and proton mass, respectively).

The potential for further tests of Lorentz invariance in space is discussed in [33]; for the electron, limits on several parameter combinations are expected using  $^{133}\text{Cs}$  and  $^{87}\text{Rb}$  clocks. However, these tests allow no limits on the components of  $E'_{jk}$ .

### III. INFLUENCE OF $\delta h$ ON SOLIDS

To first order in the changes, the influence of Lorentz violation in the electron's equation of motion on the properties of a crystal is induced by the expectation values of the Lorentz-violating contribution to the hamiltonian, that is calculated in this section. In Sec. III A, we present our ansatz for the electron wave function; the expectation value  $\langle \delta h \rangle$  is then calculated in Sec. III B.

We denote by  $(x_a)_i$ ,  $(p_a)_i$ , and  $(\sigma_a)^i$  the spatial, 3-momentum, and Pauli matrices for the  $a$ th particle. The non-relativistic single-particle hamiltonian for the  $a$ th particle is denoted  $h_a = \hat{h}_a + \delta h_a$ . The hamiltonian of the solid

$$h_{\text{all}} = \sum_a \left[ \hat{h}_a + \delta h_a \right] + \frac{1}{2} \sum_{a \neq b} \left[ \hat{h}_{a,b} + \delta h_{a,b} \right] \quad (15)$$

is the sum of  $\hat{h}_a + \delta h_a$  over all particles, plus the sum of the interaction terms  $\hat{h}_{a,b}$  over all pairs, and over  $\delta h_{a,b}$ , a possible Lorentz-violating correction to it. (The factor  $\frac{1}{2}$  corrects for the double-counting of pairs.) The Lorentz violating terms are contained in  $\delta h_a$  and  $\delta h_{a,b}$ . To first order in the changes, the resulting modifications of the properties of the solid are the sum of the modifications arising from the individual terms.

The interactions in a solid are electromagnetic. The geometry change of crystals as a consequence of the modification to the interaction term from the photonic sector of the SME [17, 18] has been treated for ionic crystals in [19]. We will not consider this term further here. In this work, we deal with the modifications due to the Lorentz violation in the electrons' equation of motion,  $\sum_a \delta h_a$ .

#### A. Wave function ansatz for the solid

According to the Bloch theorem ([34], pp. 133-141), the single-electron wave function  $\psi_a$  for the  $a$ -th electron ( $a = 1, \dots, N$ ) of a solid can be written as the product of a plane wave  $\exp\{\frac{i}{\hbar} \vec{q}_a \vec{x}_a\}$  (where  $\vec{q}_a$  is the quasi-momentum of the  $a$ th electron) and a function  $u_{\vec{q}_a}(\vec{r})$  with the period of the lattice.  $u_{\vec{q}_a}(\vec{r})$  depends on  $\vec{q}_a$ , and thus on the electron number  $a$ . To make a Fourier expansion of  $u_{\vec{q}_a}(\vec{r})$ , we note that, if  $k_{ji}$  is the  $3 \times 3$  matrix containing the primitive reciprocal lattice vectors  $\vec{k}_i$ , any reciprocal

lattice vector can be expressed as a linear combination  $n_i k_{ji}$  with some coefficients  $n_i \in \mathbb{Z}$  ([34], pp. 86-87). Therefore,

$$\psi_a = \frac{1}{\sqrt{V}} \exp \left\{ \frac{i}{\hbar} \vec{q}_a \vec{x}_a \right\} \sum_{\vec{n}} (c_{\vec{n}})_a \exp \{ -i n_j k_{ij} (x_a)_i \}, \quad (16)$$

where  $V$  is the volume of the (macroscopic) solid considered. The  $(c_{\vec{n}})_a$  are the Fourier coefficients of  $u_{\vec{q}_a}(\vec{r})$ ; they depend only on  $n_j k_{ij} - (q_a)_i$ , i.e., they can be expressed as  $c_{n_j k_{ij} - (q_a)_i}$ . The  $\vec{n}$  summation is carried out over  $\mathbb{Z}^3$ . The  $(c_n)_a$  satisfy

$$\sum_{\vec{n}} |(c_{\vec{n}})_a|^2 = 1 \quad (17)$$

because of normalization  $\langle (\psi)_a | (\psi)_a \rangle = 1$ . If we assume that the crystal has inversion symmetry, the origin of the coordinate system may be chosen such that ([34], p.137)

$$(c_{-\vec{n}})_a = (c_{\vec{n}}^*)_a. \quad (18)$$

The star denotes complex conjugation.

The normalized antisymmetric  $N$ -electron state  $\Psi^N$  ( $N$  is the total number of electrons) can be constructed from the  $N \times N$  matrix

$$(\psi) := \begin{pmatrix} \psi_1(\vec{x}_1) & \dots & \psi_1(\vec{x}_N) \\ \vdots & \ddots & \vdots \\ \psi_N(\vec{x}_1) & \dots & \psi_N(\vec{x}_N) \end{pmatrix} \quad (19)$$

as the Slater determinant [35]  $\Psi^N = \frac{1}{\sqrt{N!}} \det(\psi)$  [ $\det$  denotes the determinant of a square matrix].

## B. Calculation of matrix elements

### 1. Specifications

For a bound system in its rest frame, the expectation value of the particle momenta vanishes

$$\sum_a \langle (p_a)_i \rangle = 0. \quad (20)$$

We also assume no spin polarization, i.e., the sum of the spin expectation values

$$S^l \equiv \frac{1}{N} \sum_a \langle (\sigma_a)^l \rangle \quad (21)$$

vanishes. The case of spin polarization will be considered in the appendix. Furthermore, we assume a vanishing sum of the helicities of the electrons,

$$\sum_a \langle (p_a)_j (\sigma_a)^k \rangle = 0 \quad (22)$$

and

$$\sum_a \langle (p_a)_i (p_a)_j (\sigma_a)^k \rangle = 0. \quad (23)$$

Although situations could be imagined which violate the last two relations in spite of  $S^l = 0$ , this can be considered highly unrealistic. Therefore, the expectation values of the terms proportional to  $C_j$ ,  $D_{jk}$ , and  $F'_{jkl}$  from the hamiltonian, Eq. (3), vanish. Disregarding the constant term proportional to  $A$ ,

$$\langle (\delta h) \rangle = \frac{1}{m} E'_{ij} \sum_{a=1}^N \langle (p_a)_i (p_a)_j \rangle.$$

### 2. Calculation of $\delta h$

We now calculate the matrix element  $\langle (p_1)_i (p_1)_j \rangle$  for the first electron. Since it turns out to be independent from the electrons number (a consequence of the antisymmetry of the  $N$ -electron state  $\Psi^N$ ), the sum of the matrix elements for all electrons can then be obtained by multiplying  $\langle (p_1)_i (p_1)_j \rangle$  with the total number of electrons  $N$ . We have

$$\langle (p_1)_i (p_1)_j \rangle = \int_V \Psi^{N*} \frac{-\hbar^2 \partial^2}{\partial (x_1)_i \partial (x_1)_j} \Psi^N d^3 x_1 \dots d^3 x_N. \quad (24)$$

The integrations are carried out over the volume  $V$  of the solid.  $\Psi^N$  and  $\Psi^{N*}$  are given by Slater determinants. Evaluation of the matrix element starts by an expansion of these determinants with respect to the first column,

$$\det(\psi) = \sum_{a=1}^N (-1)^a \det(|_1 \bar{\psi}^*{}^a|), \quad (25)$$

where  $(|_1 \bar{\psi}^*{}^a|)$  denotes the  $(N-1) \times (N-1)$  minor matrix obtained from the  $N \times N$  matrix  $(\psi)$  by deleting the first column and the  $a$ -th row. The derivatives can then be carried out:

$$\langle (p_1)_i (p_1)_j \rangle = \frac{1}{N!} \sum_{a,b=1}^N (-1)^{a+b} \sum_{\vec{n}, \vec{m}} (c_{\vec{m}})_a^* (c_{\vec{n}})_b [(q_b)_i (q_b)_j + \hbar^2 n_l k_{il} n_k k_{jk} - \hbar n_k k_{ik} (q_b)_j - \hbar n_l k_{jl} (q_b)_i] \quad (26)$$

$$\times \frac{1}{V} \int_V \exp \left\{ i(x_1)_l \left[ (m_i - n_i)k_{li} + \frac{1}{\hbar} [(q_b)_l - (q_a)_l] \right] \right\} d^3 x_1 \int_V \det(|_1\bar{\psi}^{*a}) \det(|_1\bar{\psi}^b) d^3 x_2 \dots d^3 x_N.$$

Note that only the first integral in Eq. (26) contains  $\bar{x}_1$ . Using the abbreviation

$$\kappa_l = (m_i - n_i)k_{li} + \frac{1}{\hbar} [(q_b)_l - (q_a)_l], \quad (27)$$

the  $d^3 x_1$ -integration in Eq. (26) can be expressed as

$$\int_V \exp \{ i(x_1)_l \kappa_l \} d^3 x_1 = \begin{cases} V & (\kappa_l = 0), \\ 0 & (\kappa_l \neq 0). \end{cases} \quad (28)$$

Since the quasi-momenta  $(q_a)_i$  are within the first Brillouin zone ([34], p. 89),  $|(q_a)_l| \leq (\hbar/2)|n_j k_{lj}|$  for any  $n_j \in \{\mathbb{Z} \setminus 0\}$ . Thus,  $\kappa_l = 0$  only if  $n_i = m_i$  and  $(q_b)_l = (q_a)_l$ . We may assume that this holds only for  $a = b$ . That allows to carry out the  $\bar{m}$  and the  $b$  summations. We now use

$$\sum_{\bar{n}} |(c_{\bar{n}})_a|^2 n_i = 0, \quad (29)$$

which follows from Eq. (18) and eliminates the terms linear in  $n$  from the first line of Eq. (26) [36]. We define

$$(\xi_a)_{lk} := \sum_{\bar{n}} |(c_{\bar{n}})_a|^2 n_l n_k \quad (30)$$

and

$$\overline{q_i q_j} := \frac{1}{N} \sum_a (q_a)_i (q_a)_j, \quad (31)$$

the average of the quasi-momentum product  $q_i q_j$  over all electrons. We also define the average

$$\overline{\xi_{ij}} := \frac{1}{N} \sum_a (\xi_a)_{ij}. \quad (32)$$

Together with Eq. (17), this yields

$$\begin{aligned} \langle (p_1)_i (p_1)_j \rangle &= \frac{N}{N!} [\overline{q_i q_j} + \hbar^2 \overline{\xi_{lk}} k_{il} k_{jk}] \\ &\times \int_V d^3 x_2 \dots d^3 x_N \det(|_1\bar{\psi}^{*a}) \det(|_1\bar{\psi}^b) \\ &= [\overline{q_i q_j} + \hbar^2 \overline{\xi_{lk}} k_{il} k_{jk}] \langle \Psi^{N-1} | \Psi^{N-1} \rangle. \end{aligned} \quad (33)$$

To prove that  $\langle \Psi^{N-1} | \Psi^{N-1} \rangle = 1$  we expand the remaining determinants of  $(|_1\bar{\psi}^{*a})$  in terms of the column which is now the first one. The  $d^3 x_2$  integration can then be carried out. The procedure is repeated, until the  $d^3 x_N$  integration is done. Each step reduces the dimension of the Slater determinant by one and produces a factor equal to the number of electrons still involved. Taking all these factors together cancels the normalization factor  $1/(N-1)!$ . Thus, we obtain the desired result

$$\langle (p_1)_i (p_1)_j \rangle = \overline{q_i q_j} + \hbar^2 \overline{\xi_{lk}} k_{il} k_{jk}. \quad (34)$$

Since the right hand side of this result contains no reference to the electron's number, it holds for all  $a = 1, \dots, N$  electrons.

### 3. Estimating $\overline{\xi_{lk}}$

The properties of the wave function enter the momentum expectation value via  $\overline{\xi_{lk}}$  and  $\overline{q_i q_j}$ .

$\overline{\xi_{lk}}$  is an ensemble average over all electrons:

$$\overline{\xi_{lk}} = \sum_{\bar{n}} \left( \frac{1}{N} \sum_a |(c_{\bar{n}})_a|^2 n_l n_k \right) =: \sum_{\bar{n}} \overline{|c_{\bar{n}}|^2} n_l n_k, \quad (35)$$

obtained by substituting Eq. (30) into Eq. (32). A detailed evaluation of  $\overline{\xi_{lk}}$  would start from material specific Fourier coefficients  $c_{\bar{n}}$  obtained experimentally or theoretically (see, e.g. [37]). Since detailed wave-function calculations for realistic materials are notoriously difficult and would have to be performed for each individual material, it is interesting to use a relatively simple model for the Fourier coefficients. Such a model might already be quite accurate, since only the average of the absolute square  $\overline{|c_{\bar{n}}|^2}$  is required, rather than the detailed  $(c_{\bar{n}})_a$  for the individual electrons. A (possibly complicated) dependency of the  $(c_{\bar{n}})_a$  on  $\bar{n}$  can be hoped to smooth out in the averaging. The model must, however, be in accordance with the requirement that the wave function has the rotational symmetry of the lattice, i.e.  $c_{\hat{\rho}\bar{n}} \equiv c_{\bar{n}}$  if  $\hat{\rho}$  is any operator of the rotation group of the crystal ([37], pp. 469).

For such a simple model, we assume that  $\overline{|c_{\bar{n}}|} \equiv \overline{|c_{|\bar{n}|}|}$ , i.e., the average of the absolute squares of the average of the Fourier coefficients depends only on  $|\bar{n}|$ . It follows that

$$\overline{\xi_{lk}} = \gamma_{\text{mat}} \delta_{lk} \quad (36)$$

with some material dependent constant  $\gamma_{\text{mat}}$ . For determining  $\gamma_{\text{mat}}$ , we note that the average kinetic energy of an electron  $\langle T \rangle = \frac{1}{2m} \langle p_i p_j \rangle \delta_{ij}$ . From Eqs. (34), (35), and (36),

$$\langle T \rangle = \gamma_{\text{mat}} \frac{\hbar^2}{2m} \delta_{lk} k_{il} k_{jk} \delta_{ij}. \quad (37)$$

If we neglect for the moment the energy of the chemical bonding, this should correspond to the average of the kinetic energies of the atoms' valence electrons, which can be estimated using the Bohr model. The kinetic energy of an electron in the Bohr model  $T_{\text{Bohr}} = E_R Z/n^2$ . Here,  $E_R \simeq 13.6 \text{ eV}$  is the Rydberg energy,  $Z$  the charge number of the atom core, and  $n$  the principal quantum number. Thus, the kinetic energy from the Bohr model, averaged over the electrons within the atoms of the molecule,

$$\overline{T_{\text{Bohr}}} = \frac{1}{N_{e,m}} \sum_{k=1}^{N_{e,m}} v_k \frac{E_R Z_k}{n_k^2} \quad (38)$$

where  $N_{e,m}$  gives the number of valence electrons per molecule. The index  $k$  enumerates the atoms of the molecule and  $v_k, n_k$ , and  $Z_k$  are the valence, principal quantum number, and charge number, respectively, of the atom  $k$ . Note that  $Z_k = v_k$ , since in an atom with  $v$  valence electrons, the charge number of the atom cores and the inner shell electrons is  $Z = v$ . For example, in quartz,  $\text{SiO}_2$ , there is one Si atom with  $v = 4$ ,  $n = 3$  and two O atoms with  $v = 2$  and  $n = 2$ . Thus, for example,

$$\overline{(T_{\text{Bohr}})}_{\text{quartz}} = \frac{E_R}{8} \left( 1 \frac{4^2}{3^2} + 2 \frac{2^2}{2^2} \right) = \frac{17}{36} E_R. \quad (39)$$

Comparing this to Eq. (37), we obtain the material specific values  $\gamma_{\text{mat}}$  given in Tab. I.

The model can be refined by taking into account the energy of the chemical bonding, which leads to an increase of the actual kinetic energy of the electrons. The so called enthalpy of formation  $\Delta_f H^0$  gives the enthalpy for the formation of the crystal from the elements in their usual state at standard conditions (room temperature and pressure), e.g., solid or diatomic ( $\text{O}_2$ , for example). The Bohr model, however, predicts the energy of the unbound atoms. That means, the change  $T - T_{\text{Bohr}}$  between the sum of the kinetic energy of the valence electrons of the free atoms  $T_{\text{Bohr}}$  and the sum of their kinetic energy in the molecule  $T$  is the difference of  $\Delta_f H^0$  and the applicable enthalpies of sublimation  $\Delta_{\text{subl}} H^0$  or dissociation  $\Delta_{\text{diss}} H^0$  of the elements. For sapphire,  $\text{Al}_2\text{O}_3$ , for example,

$$\begin{aligned} \Delta_f H^0(\text{Al}_2\text{O}_3) &= 16.8 \text{ eV} \\ -\Delta_{\text{subl}} H^0(2\text{Al}) &= -2 \times 3.0 \text{ eV} \\ -\Delta_{\text{diss}} H^0(3\text{O}) &= -3 \times 2.5 \text{ eV} \\ \hline T - T_{\text{Bohr}} &= 3.3 \text{ eV}, \end{aligned}$$

or about 5% of  $T_{\text{Bohr}} = 68 \text{ eV}$ . This would lead to a 5% increase of the factor  $\gamma_{\text{mat}}$ . This indicates that the energy of the chemical bonding is, for our purposes, negligible.

The ultimate refinement of the model would be the insertion of material specific Fourier coefficients  $c_{\vec{n}}$  into Eq. (35). The precision of the model would then approach the limitations of the Bloch ansatz for the wave function itself, which is based on a mean field model for the electron-electron interactions. Such a detailed model is, however, beyond the scope of the present work.

#### 4. Result

The expectation value of the Lorentz-violating correction to the single particle hamiltonian  $\sum_a \delta h_a$  can be obtained from Eq. (34) by multiplying with the number of electrons. Inserting  $\xi_{lk}$  as obtained in the previous section into Eq. (34), we obtain

$$\langle \delta h \rangle = \frac{N}{m} E'_{ij} (\overline{q_i q_j} + \gamma_{\text{mat}} \hbar^2 \delta_{lk} k_{il} k_{jk}). \quad (40)$$

The quasi-momenta  $|\vec{q}_a|$  are restricted to the first Brillouin zone,  $|\vec{q}| < \frac{\hbar}{2} |\vec{k}_j|$ . Most electrons, however, will have a quasi-momentum lower than this maximum value, so that the average  $\overline{q_i q_j}$  is a relatively small contribution to  $\langle \delta h \rangle$ . If we neglect it, we obtain the final result

$$\langle \delta h \rangle = N \gamma_{\text{mat}} \frac{\hbar^2}{m} E'_{ij} \delta_{lk} k_{il} k_{jk}. \quad (41)$$

$\delta_{lk} k_{il} k_{jk}$  is symmetric in the indices  $i$  and  $j$ . This result will be used in the next section to compute the geometry change of the crystal caused by Lorentz violation in the electrons' equation of motion.

## IV. CHANGE OF CRYSTAL GEOMETRY

The direct lattice vectors  $\vec{l}_a$  contained in the matrix  $l_{ia}$  determine the structure of the lattice without Lorentz violation. Lorentz violation will cause a change  $\tilde{l}_{ia}$  of the crystal geometry, i.e., the lattice vectors are now given by  $l_{ia} + \tilde{l}_{ia}$ . To calculate it, we adjust  $\tilde{l}_{ia}$  such as to minimize the total energy of the lattice

$$U = U_0(l_{ia} + \tilde{l}_{ia}) + \langle \delta h(l_{ia} + \tilde{l}_{ia}) \rangle. \quad (42)$$

The first term is the conventional total energy of the lattice without Lorentz violation. It can be expressed as

$$U_0(l_{ia} + \tilde{l}_{ia}) = U_0(l_{ia}) + U_{\text{elast}}(\tilde{l}_{ia}) + U_c \quad (43)$$

where  $U_c$  is a constant and  $U_{\text{elast}}$  is the elastic energy connected to a distortion of the lattice. If  $\tilde{l}_{ia} = 0$ , the elastic energy  $U_{\text{elast}} = 0$ . The total energy is thus given by

$$U = U_0(l_{ia}) + U_{\text{elast}}(\tilde{l}_{ia}) + \langle \delta h(l_{ia} + \tilde{l}_{ia}) \rangle. \quad (44)$$

The correction  $\tilde{l}_{ia}$  is found by setting to zero the derivative:

$$\frac{\partial U}{\partial \tilde{l}_{jb}} = \frac{\partial U_{\text{elast}}}{\partial \tilde{l}_{jb}} + \frac{\partial \langle \delta h(l_{ia} + \tilde{l}_{ia}) \rangle}{\partial \tilde{l}_{jb}} = 0. \quad (45)$$

To explicitly calculate  $\tilde{l}_{jb}$ , we have to express the contributions to  $U$  in terms of  $\tilde{l}_{jb}$ . We will do so for  $\langle \delta h \rangle$  in Sec. IV A and in Sec. IV B for  $U_{\text{elast}}$ . In Sec. IV C, the total energy per unit cell thus obtained is minimized and the geometry change as expressed by a strain tensor  $e_{ij}$  is calculated.

### A. Dependence of $\delta h$ on $\tilde{l}_{ia}$

The change of the hamiltonian's expectation value  $\langle \delta h \rangle$ , Eq. (41) depends on the geometry via the reciprocal lattice vectors  $k_{ij}$ , for which we have the relation ([34], p. 87),

$$l_{ij} k_{ik} = 2\pi \delta_{jk}, \quad (46)$$

and therefore  $l_{ij}k_{nj} = 2\pi\delta_{in}$ . If we substitute  $l_{ij} + \tilde{l}_{ij}$  and  $k_{jk} + \tilde{k}_{jk}$ , with  $\tilde{l}_{ij} \ll l_{ij}$  and  $\tilde{k}_{jk} \ll k_{jk}$ , we obtain

$$(l_{ij} + \tilde{l}_{ij})(k_{ik} + \tilde{k}_{ik}) = 2\pi\delta_{jk} \quad (47)$$

or

$$l_{ij}k_{ik} + l_{ij}\tilde{k}_{ik} + \tilde{l}_{ij}k_{ik} + \tilde{l}_{ij}\tilde{k}_{ik} = 2\pi\delta_{jk}. \quad (48)$$

The first term on the l.h.s. cancels with the r.h.s due Eq. (46); we neglect the second order term on the l.h.s., and obtain

$$l_{ij}\tilde{k}_{ik} + \tilde{l}_{ij}k_{ik} = 0. \quad (49)$$

Multiplying with  $k_{nj}$  and using Eq. (46) again,

$$\tilde{k}_{nk} = -\frac{1}{2\pi}k_{nj}\tilde{l}_{ij}k_{ik}. \quad (50)$$

We can now substitute  $k_{ij} + \tilde{k}_{ij}$  into Eq. (41) to obtain  $\delta h(\tilde{l}_{ab})$ :

$$\begin{aligned} \delta h(\tilde{l}_{ab}) &= N\gamma_{\text{mat}}\frac{\hbar^2}{m}\delta_{lk}\left(k_{il} - \frac{1}{2\pi}k_{ia}\tilde{l}_{ba}k_{bl}\right) \\ &\times\left(k_{jk} - \frac{1}{2\pi}k_{ja}\tilde{l}_{ba}k_{bk}\right)E'_{ij} \end{aligned} \quad (51)$$

$$\begin{aligned} &= \text{const} - \gamma_{\text{mat}}\frac{N\hbar^2}{2\pi m}E'_{ij} \\ &\times(k_{ia}\tilde{l}_{ba}k_{bk}k_{jk} + k_{ja}\tilde{l}_{ba}k_{bk}k_{ik}). \end{aligned} \quad (52)$$

The  $\text{const} = N\gamma_{\text{mat}}\frac{\hbar^2}{m}E'_{ij}\delta_{lk}k_{il}k_{jk}$  does not depend on  $\tilde{l}_{ab}$ . A term of order  $E'_{ij}(\tilde{l}_{ab})^2$  has been neglected.

## B. Elastic energy

The elastic energy is given as [38]

$$U_{\text{elast}} = \frac{1}{2}\lambda_{ijkl}e_{ij}e_{kl}V, \quad (53)$$

where  $\lambda_{ijkl}$  is the elastic modulus,  $V$  the volume considered, and

$$e_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \quad (54)$$

is the strain tensor, where  $u_i$  is the displacement of a volume element at some location  $x_i$ . For  $i = j$ ,  $u_{ij}$  represents the relative change of length in  $x_i$ -direction, and for  $i \neq j$ , it represents the change of the right angle between lines originally pointing in  $x_i$  and  $x_j$  direction.

To express the elastic energy in terms of  $\tilde{l}_{ij}$ , we note that the location  $x_b$  of a point of the direct lattice can be expressed as a linear combination of the primitive lattice vectors

$$x_b = \eta_a l_{ba}, \quad (55)$$

with some coefficients  $\eta_a \in \mathbb{N}$ . Multiplying this equation by  $k_{bc}$  and using Eq. (46), we obtain

$$\eta_c = \frac{1}{2\pi}k_{bc}x_b. \quad (56)$$

If  $l_{ba}$  is shifted to  $l_{ba} + \tilde{l}_{ba}$ , the lattice point originally at  $x_b$  will be shifted to  $x_b + u_b$ , where

$$u_b = \eta_a \tilde{l}_{ba} = \frac{1}{2\pi}k_{da}x_d \tilde{l}_{ba}. \quad (57)$$

Therefore, we have

$$\frac{\partial u_d}{\partial x_c} = \frac{1}{2\pi}k_{ca}\tilde{l}_{da} \quad (58)$$

or

$$e_{dc} = \frac{1}{4\pi}\left(k_{da}\tilde{l}_{ca} + k_{ca}\tilde{l}_{da}\right). \quad (59)$$

This can now be used to express the elastic energy in terms of  $\tilde{l}_{ab}$ :

$$U_{\text{elast}} = \frac{1}{2}\lambda_{ijkl}\frac{1}{4\pi}(k_{ia}\tilde{l}_{ja} + k_{ja}\tilde{l}_{ia})\frac{1}{4\pi}(k_{lb}\tilde{l}_{kb} + k_{kb}\tilde{l}_{lb})V. \quad (60)$$

Some manipulation of indices using  $\lambda_{abcd} = \lambda_{bacd} = \lambda_{cdab}$  leads to the more simple form

$$U_{\text{elast}} = \frac{V}{8\pi^2}\lambda_{ijkl}k_{ia}\tilde{l}_{ja}k_{lb}\tilde{l}_{kb}. \quad (61)$$

## C. Minimizing the total energy per unit cell

Summing up the contributions, we find for the energy change per unit cell (leaving out the constant terms)

$$\begin{aligned} U &= |\det(l_{ij})|\frac{1}{8\pi^2}\lambda_{ijkl}k_{ia}\tilde{l}_{ja}k_{lb}\tilde{l}_{kb} - \gamma_{\text{mat}}\frac{N\hbar^2}{2\pi m} \\ &\times E'_{ij}(k_{ia}\tilde{l}_{ba}k_{bk}k_{jk} + k_{ja}\tilde{l}_{ba}k_{bk}k_{ik}) \end{aligned} \quad (62)$$

were  $V = |\det(l_{ij})|$ , the volume of a unit cell, and  $N = N_{e,u}$  the number of valence electrons per unit cell have been inserted (not to be confused with  $N_{e,m}$  the corresponding number per molecule). The inner-shell electrons are assumed not to influence the crystal geometry. A minimum is found, when

$$\frac{\partial U}{\partial \tilde{l}_{mn}} = 0. \quad (63)$$

After some manipulation, the derivative can be expressed as

$$\begin{aligned} \frac{\partial U}{\partial \tilde{l}_{mn}} &= \frac{|\det(l_{ij})|}{4\pi^2}\lambda_{imkl}k_{in}k_{lb}\tilde{l}_{kb} - \gamma_{\text{mat}}\frac{N_{e,u}\hbar^2}{2\pi m} \\ &\times E'_{ij}(k_{in}k_{mk}k_{jk} + k_{jn}k_{mk}k_{ik}) = 0. \end{aligned} \quad (64)$$

We denote  $E'_{(ij)} = \frac{1}{2}(E'_{ij} + E'_{ji})$  the symmetric part of the tensor  $E'_{ij}$ . The last equation can be simplified a bit by multiplying with  $l_{pn}$ :

$$\lambda_{pmkl}k_{lb}\tilde{l}_{kb} - \gamma_{\text{mat}} \frac{4\pi\hbar^2 N_{e,u}}{|\det(l_{ij})|m} E'_{(pj)} k_{mk} k_{jk} = 0. \quad (65)$$

For solving this for  $\tilde{l}$ , we need the inverse  $\mu_{abkl}$  (called the compliance tensor) of  $\lambda_{abcd}$ , defined by

$$\mu_{abkl}\lambda_{abcd} = \delta_{kc}\delta_{dl}. \quad (66)$$

Multiplying Eq. (65) with  $\mu_{depm}$  gives

$$k_{eb}\tilde{l}_{db} = \gamma_{\text{mat}} \frac{4\pi N_{e,u}}{|\det(l_{ij})|} \frac{\hbar^2}{m} E'_{(pj)} \mu_{depm} k_{mk} k_{jk} \quad (67)$$

and a further multiplication by  $l_{es}$  yields

$$\tilde{l}_{ds} = \gamma_{\text{mat}} \frac{2\hbar^2 N_{e,u}}{m|\det(l_{ij})|} E'_{(pj)} \mu_{depm} l_{es} k_{mk} k_{jk}. \quad (68)$$

The strain tensor can be calculated from this result using Eq. (59) as

$$e_{dc} = \tilde{\mathcal{B}}_{dcpj} E'_{(pj)} \quad (69)$$

with

$$\tilde{\mathcal{B}}_{dcpj} = \gamma_{\text{mat}} \frac{2N_{e,u}\hbar^2}{m|\det(l_{ij})|} \mu_{dcmp} k_{mk} k_{jk}. \quad (70)$$

This has been simplified by using Eq. (46). Since for Eq. (69), this is multiplied with the symmetric  $E'_{(jp)}$ , only the part  $\mathcal{B}_{dcpj} = \frac{1}{2}(\tilde{\mathcal{B}}_{dcpj} + \tilde{\mathcal{B}}_{dcjp})$  that is symmetric in  $j$  and  $p$

$$\mathcal{B}_{dcjp} = \gamma_{\text{mat}} \frac{N_{e,u}\hbar^2}{m|\det(l_{ij})|} (\mu_{dcmp} k_{mk} k_{jk} + \mu_{dcmj} k_{mk} k_{pk}) \quad (71)$$

is used. The resulting strain tensor

$$e_{dc} = \mathcal{B}_{dcpj} E'_{pj} \quad (72)$$

is given by the  $3 \times 3$  Lorentz violation tensor  $E'_{pj}$  and a tensor  $\mathcal{B}_{dcpj}$ , which gives the sensitivity of the material geometry change to Lorentz violation in the electron sector of the SME. This is the desired result of this section.

### 1. General properties of the sensitivity tensor $\mathcal{B}_{dcpj}$ and conventions

The sensitivity tensor has the symmetries

$$\mathcal{B}_{dcjp} = \mathcal{B}_{cdjp} = \mathcal{B}_{dcpj}. \quad (73)$$

In general, however,  $\mathcal{B}_{dcjp} \neq \mathcal{B}_{jpd}$ . It has, therefore, at most 36 independent elements, the number of which

is reduced for a symmetric crystal. For a compact presentation of the material specific results in the following sections, we will arrange these into a  $6 \times 6$  matrix, that allows to express Eq. (69) as a 6 dimensional matrix equation

$$e_{\Gamma} = \mathcal{B}_{\Gamma\Xi} E'_{\Xi}. \quad (74)$$

We therefore arrange the six independent elements of  $e_{dc}$  and  $E'_{(bj)}$  as the vectors

$$e_{\Gamma} = (e_{xx}, e_{yy}, e_{zz}, e_{yz}, e_{zx}, e_{xy}), \quad (75)$$

$$E'_{\Gamma} = (E'_{xx}, E'_{yy}, E'_{zz}, E'_{yz}, E'_{zx}, E'_{xy}) \quad (76)$$

[the capital greek indices run from 1...6] and define the sensitivity matrix

$$\mathcal{B} = \begin{pmatrix} \mathcal{B}_{1111} & \mathcal{B}_{1122} & \mathcal{B}_{1133} & 2\mathcal{B}_{1123} & 2\mathcal{B}_{1131} & 2\mathcal{B}_{1112} \\ \mathcal{B}_{2211} & \mathcal{B}_{2222} & \mathcal{B}_{2233} & 2\mathcal{B}_{2223} & 2\mathcal{B}_{2231} & 2\mathcal{B}_{2212} \\ \mathcal{B}_{3311} & \mathcal{B}_{3322} & \mathcal{B}_{3333} & 2\mathcal{B}_{3323} & 2\mathcal{B}_{3331} & 2\mathcal{B}_{3312} \\ \mathcal{B}_{2311} & \mathcal{B}_{2322} & \mathcal{B}_{2333} & 2\mathcal{B}_{2323} & 2\mathcal{B}_{2331} & 2\mathcal{B}_{2312} \\ \mathcal{B}_{3111} & \mathcal{B}_{3122} & \mathcal{B}_{3133} & 2\mathcal{B}_{3123} & 2\mathcal{B}_{3131} & 2\mathcal{B}_{3112} \\ \mathcal{B}_{1211} & \mathcal{B}_{1222} & \mathcal{B}_{1233} & 2\mathcal{B}_{1223} & 2\mathcal{B}_{1231} & 2\mathcal{B}_{1212} \end{pmatrix}. \quad (77)$$

The factors of 2 account for the double-counting of the non-diagonal elements of  $E'_{(pj)}$  in the tensor equation Eq. (69).

### 2. Sensitivity matrix for isotropic materials

Let us first consider isotropic materials that have no preferred crystal orientation, i.e. crystals of cubic structure and non-crystalline (fused) materials which consist of a large number of small crystals oriented statistically. Cubic materials have one single lattice constant  $a$ ; the matrix of the primitive direct lattice vectors is given by  $l_{ij} = a\delta_{ij}$ . According to Eq. (46), the matrix of the reciprocal lattice vectors is given by  $k_{ij} = (2\pi/a)\delta_{ij}$ . In the appendix, it is described how to obtain the compliance constants  $\mu_{abcd}$  from the elasticity constants that are tabulated for various materials in the literature, e.g. [39]. Inserting into Eqs. (71,77), we obtain the sensitivity matrix  $\mathcal{B}$ . It is of the structure

$$\mathcal{B} = \begin{pmatrix} \mathcal{B}_{11} & \mathcal{B}_{12} & \mathcal{B}_{12} & 0 & 0 & 0 \\ \mathcal{B}_{12} & \mathcal{B}_{11} & \mathcal{B}_{12} & 0 & 0 & 0 \\ \mathcal{B}_{12} & \mathcal{B}_{12} & \mathcal{B}_{12} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathcal{B}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathcal{B}_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathcal{B}_{44} \end{pmatrix}. \quad (78)$$

For cubic crystals, the non-zero values

$$\mathcal{B}_{11} = \xi/(a^2)C_{11},$$

$$\mathcal{B}_{12} = \xi/(a^2)C_{12},$$

$$\mathcal{B}_{44} = \xi/(2a^2)C_{44},$$

where

$$\xi = \gamma_{\text{mat}} \frac{8\pi^2 N_{e,u} \hbar^2}{m |\det(l_{ij})|} \quad (79)$$

and  $C_{\Gamma\Xi}$  are the elements of the  $6 \times 6$  compliance matrix, Eq. (B9). From symmetry arguments, this is also the structure of the  $\mathcal{B}$  matrix for non crystalline materials without a preferred orientation. The elements of this matrix for some cubic and/or fused materials are given in table I. The values for fused quartz and sapphire have been calculated from the values of the crystalline materials (to be calculated below) as averages over crystal orientations.

### 3. Sensitivity matrix for trigonal crystals

Quartz and Sapphire are of trigonal structure and are frequently used in cavity experiments. Therefore, we also consider the trigonal case here. The matrix of the primitive direct lattice vectors can be chosen as

$$l_{ij} = \begin{pmatrix} a/2 & a/2 & 0 \\ \sqrt{3}a/2 & -\sqrt{3}a/2 & 0 \\ 0 & 0 & c \end{pmatrix} \quad (80)$$

where  $a$  and  $c$  are the two lattice constants. We calculate the inverse  $k_{ij}$ ; the product

$$k_{ik} k_{jk} = 4\pi^2 \begin{pmatrix} 2/a^2 & 0 & 0 \\ 0 & 2/(3a^2) & 0 \\ 0 & 0 & 1/c^2 \end{pmatrix} \quad (81)$$

turns out to be a diagonal matrix. Trigonal crystals have six independent compliance constants and two lattice constants, which makes 8 independent components for the  $\mathcal{B}$ -matrix. It has the structure

$$\mathcal{B} = \begin{pmatrix} \mathcal{B}_{11} & \mathcal{B}_{12} & \mathcal{B}_{13} & \mathcal{B}_{14} & 0 & 0 \\ 3\mathcal{B}_{12} & \frac{1}{3}\mathcal{B}_{11} & \mathcal{B}_{13} & -\mathcal{B}_{14} & 0 & 0 \\ \mathcal{B}_{31} & \frac{1}{3}\mathcal{B}_{31} & \mathcal{B}_{33} & 0 & 0 & 0 \\ \mathcal{B}_{41} & -\frac{1}{3}\mathcal{B}_{41} & 0 & \mathcal{B}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathcal{B}_{55} & \frac{2}{3}\mathcal{B}_{41} \\ 0 & 0 & 0 & 0 & \mathcal{B}_{55} & \mathcal{B}_{66} \end{pmatrix} \quad (82)$$

with

$$\begin{aligned} \mathcal{B}_{55} &= \mathcal{B}_{44} + \frac{1}{3}\mathcal{B}_{41}, \\ \mathcal{B}_{66} &= \frac{1}{3}\mathcal{B}_{11} - \mathcal{B}_{12}. \end{aligned}$$

The matrix elements are explicitly

$$\begin{aligned} \mathcal{B}_{11} &= 2\xi/(a^2)C_{11}, \\ \mathcal{B}_{12} &= 2\xi/(3a^2)C_{12}, \\ \mathcal{B}_{13} &= \xi/(c^2)C_{13}, \end{aligned}$$

TABLE I: Elements of the sensitivity matrix for fused and/or cubic materials. fq denotes fused quartz, fs fused sapphire, C denotes diamond. Materials for which three elements of  $\mathcal{B}$  are given are isotropic; the coefficients should be inserted into Eq. (78). The other materials are trigonal; the coefficients for these are to be inserted into Eq. (82).

| Mat.                           | $\gamma_{\text{mat}}$ | $\mathcal{B}_{11}$ | $\mathcal{B}_{12}$ | $\mathcal{B}_{13}$ | $\mathcal{B}_{14}$ | $\mathcal{B}_{31}$ | $\mathcal{B}_{33}$ | $\mathcal{B}_{41}$ | $\mathcal{B}_{44}$ |
|--------------------------------|-----------------------|--------------------|--------------------|--------------------|--------------------|--------------------|--------------------|--------------------|--------------------|
| fq                             | 0.38                  | 0.77               | -0.09              | -                  | -                  | -                  | -                  | -                  | 0.57               |
| fs                             | 0.29                  | 0.06               | -0.01              | -                  | -                  | -                  | -                  | -                  | 0.05               |
| Si                             | 0.50                  | 2.51               | -0.70              | -                  | -                  | -                  | -                  | -                  | 2.05               |
| C                              | 1.16                  | 5.77               | -0.59              | -                  | -                  | -                  | -                  | -                  | 5.35               |
| Al <sub>2</sub> O <sub>3</sub> | 0.29                  | 0.14               | -0.01              | -0.00              | 0.02               | -0.02              | 0.01               | 0.01               | 0.04               |
| SiO <sub>2</sub>               | 0.38                  | 1.41               | -0.07              | -0.06              | 0.35               | -0.14              | 0.44               | 0.25               | 0.41               |

$$\begin{aligned} \mathcal{B}_{14} &= \xi[1/(3a^2) + 1/(2c^2)]C_{14}, \\ \mathcal{B}_{31} &= 2\xi/(a^2)C_{13}, \\ \mathcal{B}_{33} &= \xi/(c^2)C_{33}, \\ \mathcal{B}_{41} &= \xi/(a^2)C_{14}, \\ \mathcal{B}_{44} &= \xi[1/(6a^2) + 1/(4c^2)]C_{44}. \end{aligned}$$

$C_{\Gamma\Xi}$  are the elements of the compliance matrix given in Eq. (B9). Numerical values of  $\mathcal{B}_{\Gamma\Xi}$  for quartz and sapphire are given in Tab. I. The matrix  $\mathcal{B}$  is not symmetrical; the elements of the first column are generally the highest in this matrix, i.e., the geometry change of trigonal materials is most sensitive to the  $xx$  element of the Lorentz violation parameters  $E'_{(ij)}$ . This is because the direct lattice vector components in  $x$ -direction are a factor  $\sqrt{3}$  smaller than the  $y$  components. Hence, the wave function of the electrons oscillate faster in  $x$  direction, i.e. the  $\langle p_x \rangle$  momentum component is larger. Since the influence of Lorentz violation is given by the  $\langle p_i p_j \rangle$  matrix element, this means a higher influence of the  $x$ -component of the Lorentz violation coefficients  $E'_{(ij)}$ .

High elastic constants decrease the values of  $\mathcal{B}$  so that crystals of high stiffness (such as sapphire) should show lower values of  $\mathcal{B}$ . However, in some cases (particularly diamond), this is outweighed by small dimensions of the unit cell (that imply high momentum expectation values due to short period of the electron wave functions) and a large number of electrons per unit cell.

## V. EXPERIMENTS

Here, we discuss the application of our results to extract limits on Lorentz violation in the electrons' equation of motion from experiments.

### A. Lorentz violation signal in cavity experiments

As discussed in the introduction, Lorentz violation may affect the resonance frequency of a cavity  $\nu$  through a

variation of  $c$  and  $L$ :

$$\frac{\delta\nu}{\nu_0} = \frac{\delta c}{c_0} - \frac{\delta L}{L_0}. \quad (83)$$

Here,  $\nu_0$ ,  $c_0$ , and  $L_0$  are quantities in absence of Lorentz violation. For cavity experiments, we have to consider both Lorentz violation in electrodynamics as well as in the electrons' equation of motion. The influence of Lorentz violation in electrodynamics leads to a frequency change  $\delta_{\text{EM}}\nu$  that is mainly caused by a variation of the velocity of light,  $\delta_{\text{EM}}c$  [17, 18], and a small material-dependent contribution due a length change  $\delta_{e-L}$ , that is usually negligible [19]. Lorentz violation in the electrons' equation of motion affects solely  $L$ . This leads to a frequency change  $\delta_{e-\nu}$ , so that

$$\delta\nu = \delta_{\text{EM}}\nu + \delta_{e-\nu}. \quad (84)$$

For example, if the cavity axis is parallel to the  $z$ -axis of the crystal,

$$-\frac{\delta_{e-\nu}}{\nu_0} = \frac{\delta L_z}{L_{z,0}} \equiv e_3. \quad (85)$$

From Eq. (74),  $e_3 = \mathcal{B}_{3\Xi} E'_{\Xi}$ .

### B. Limits from previous experiments

Cavity experiments have been performed repeatedly as tests of Lorentz violation in electrodynamics [9, 10, 11, 12, 13, 14, 15]. It is interesting to estimate the level of the limits on  $c_{\mu\nu}$  resulting from these experiments. Since none of them were done with a setup optimized for obtaining separate bounds on Lorentz violation in electrodynamics and in the electrons' equation of motion (see below), we have to use an assumption that simplifies the analysis, so we can work with the published data only. To obtain a sharp upper limit, we have to compare two experiments of high precision that used different cavity materials.

Müller *et al.* [15] performed a Michelson-Morley experiment using two sapphire (s) cavities subject to Earth's rotation. The cavity axes were parallel to the crystals  $c$ -axis. Since for such cavities, the elements of  $\mathcal{B}_{3\Xi}^s$  giving the sensitivity to Lorentz violation in the electronic sector are relatively low, we neglect the effect on Lorentz violation in the electrons' equation of motion for this experiment, i.e., we view the experiment as a pure test of Lorentz violation in electrodynamics. Due to Earth's rotation with the angular frequency  $\omega_{\oplus} \simeq 2\pi/23\text{h}56\text{min}$  and Earth's orbit with  $\Omega_{\oplus} = 2\pi/1\text{year}$ , Lorentz violation in electrodynamics leads to a time-dependency of the frequency difference between the cavities that has Fourier components at 6 frequencies that are linear combinations of  $\omega_{\oplus}$  and  $\Omega_{\oplus}$ . The experiment gives individual bounds on the amplitudes of these Fourier components. At  $2\omega_{\oplus}$  and  $2(\omega_{\oplus} \pm \Omega_{\oplus})$ , the bounds are below  $4 \times 10^{-15}$ .

Brillet and Hall [9] used a single fused quartz (fq) cavity (actually, "ultra-low expansion" glass ceramics, ULE) on a turntable rotating at  $\omega_t$ . Frequency measurement was accomplished by comparison to a stationary  $\text{CH}_4$  standard. Since in a single-cavity setup, the same Lorentz violation in electrodynamics leads to half the frequency variation compared to a two-cavity setup, the experiment of Müller *et al.* excludes signals from Lorentz violation in electrodynamics larger than  $2 \times 10^{-15}$  for this experiment. We may thus view this experiment as a measurement of

$$\frac{\delta_{e-\nu}}{\nu_0} = \mathcal{B}_{3\Xi}^{fq} E'_{\Xi}. \quad (86)$$

The indices  $\Xi$  denote components in the cavity frame of reference. In accordance with [17, 18, 23], we define the  $x$  axis of the laboratory frame as the north-south axis, the  $y$  axis as the east-west axis, and the  $z$  axis as pointing upwards. The turntable rotated in the  $xy$ -plane [9]. We define the cavity frame  $\bar{z}$  axis parallel to the  $z$  axis, the  $\bar{x}$  axis parallel to the cavity axis. A calculation of the hypothetical signal starts from transforming  $c_{\mu\nu}$  as given in the sun-centered standard frame into the laboratory frame, as described in [17, 18, 23]. A further rotation around the laboratory  $z$  axis gives the quantities  $c_{\bar{\mu}\bar{\nu}}$  in the cavity frame, from which  $E'_{\bar{i}\bar{j}}$  follows from Eq. (8). Due to the rotations, the hypothetical signal becomes time-dependent and is given by (assuming that at  $T_{\oplus} = 0$ , the cavity axis coincides with the  $X$  axis, and neglecting terms proportional to Earth's orbital velocity  $\beta_{\oplus} \sim 10^{-4}$ )

$$\begin{aligned} \frac{\delta\nu}{\nu} = & C(2, 0, 0) \cos 2\omega_t T_{\oplus} + S(2, 2, 0) \sin(2\omega_t + 2\omega_{\oplus}) T_{\oplus} \\ & + C(2, 2, 0) \cos(2\omega_t + 2\omega_{\oplus}) T_{\oplus} + \mathcal{A} + \mathcal{O}(\beta_{\oplus}^2), \end{aligned} \quad (87)$$

where  $\mathcal{A}$  denotes Fourier components at other frequencies, for which no experimental results are published in [9]. The sine component at  $2\omega_t$  vanishes. The coefficients are

$$\begin{aligned} C(2, 0, 0) &= -\frac{1}{4}(\mathcal{B}_{11}^{fq} - \mathcal{B}_{12}^{fq}) \sin^2 \chi_B (c_{XX} + c_{YY} - 2c_{ZZ}) \\ &\simeq -0.13 (c_{XX} + c_{YY} - 2c_{ZZ}), \\ S(2, 2, 0) &= \cos^4 \frac{\chi_B}{2} (\mathcal{B}_{11}^{fq} - \mathcal{B}_{12}^{fq}) c_{(XY)} \\ &\simeq 0.58 c_{(XY)}, \\ C(2, 2, 0) &= \frac{1}{2} \cos^4 \frac{\chi_B}{2} (\mathcal{B}_{11}^{fq} - \mathcal{B}_{12}^{fq}) (c_{YY} - c_{XX}) \\ &\simeq 0.29 (c_{YY} - c_{XX}). \end{aligned}$$

$\chi_B$  denotes the colatitude of Boulder,  $\chi_B \simeq 50^\circ$ .  $\mathcal{B}_{11}^{fq}$  and  $\mathcal{B}_{12}^{fq}$  are given in Tab. I. From the experiment, an amplitude at  $2\omega_t$  of  $\sim 2 \times 10^{-13}$  is found, attributed to a slight tilt in the horizontal alignment of the turntable. In principle, a hypothetical Lorentz violation signal at  $2\omega_t$  cannot be separated in the analysis from a signal caused by such tilt. However, if we consider an exact cancellation

between a strong Lorentz violation signal and a strong tilt signal improbable, we obtain a rough order-of-magnitude bound on  $|c_{XX} + c_{YY} - 2c_{ZZ}|$  at a level of about  $10^{-12}$ . The measured upper limit on the amplitude of the component of the hypothetical signal at  $2(\omega_t + \omega_\oplus)$  (which can be distinguished from a tilt generated signal in the Fourier analysis) is  $4 \times 10^{-15}$ . Adding in quadrature the maximum possible contribution from Lorentz violation in electrodynamics according to the result of [15],  $2 \times 10^{-15}$ , we obtain  $\sqrt{S(2, 2, 0)^2 + C(2, 2, 0)^2} \lesssim 4.5 \times 10^{-15}$ . This gives the limits

$$\begin{aligned} |c_{XY}| &\lesssim 8 \times 10^{-15}, \\ |c_{XX} - c_{YY}| &\lesssim 1.6 \times 10^{-14}. \end{aligned} \quad (88)$$

Given the small magnitude of  $\mathcal{B}_{3\Xi}^s$ , these values would indeed lead to negligible contributions to the experiment of Müller *et al.*, so our above assumptions seem reasonable.

### C. Optimized setups

To obtain clean separate bounds on Lorentz violation in electrodynamics and the electrons' equation of motion, without using the above assumptions, a dedicated experiment is desirable. One could, for example, compare the resonance frequencies  $\nu_{fq}$  and  $\nu_s$  of a cavity made from fused quartz and one from crystalline sapphire, with the cavity axis parallel to the crystal  $z$  axis, for example. This seems to be a realistic scenario, since such cavities have been used in experiments and proved to be of high stability [9, 10, 11, 14, 15, 40, 41]. The signal for Lorentz violation would be the frequency difference  $\nu_s - \nu_{fq}$ . If a parallel arrangement of cavities would be chosen, the influence of Lorentz violation in electrodynamics could be eliminated, and a clean bound on some components of  $E'_{jk}$  could be extracted,

$$\frac{\nu_s - \nu_q}{\nu} = (\mathcal{B}_{3\Xi}^{fq} - \mathcal{B}_{3\Xi}^s)E'_{\Xi}. \quad (89)$$

Here,  $\nu \simeq \nu_s \simeq \nu_q$  is the average frequency. An accuracy level of below one part in  $10^{15}$  in frequency comparisons of cavities made from quartz [40] and sapphire [15] has been demonstrated in the laboratory. Thus, placing bounds of a few parts in  $10^{15}$  on the components of  $E'_{JK}$  that dominate the signal seems feasible. A contribution of the time-components  $c_{(0J)}$  to the signal arises if one takes into account the laboratory velocity given by the velocity  $\beta_\oplus \sim 10^{-4}$  of Earth's orbit and  $0 \leq \beta_L \lesssim 1.5 \times 10^{-6}$  due to Earth's rotation (depending on the geographical latitude). The Lorentz transformations between the sun-centered inertial reference frame and the laboratory frame lead to additional Fourier components of the signal that are proportional to  $c_{(0J)}$  and either  $\beta_\oplus$  or  $\beta_L$ . In a Fourier analysis of a sufficiently long timetrace, the Fourier components can be resolved and individual limits on almost all components of  $c_{\mu\nu}$  (only  $c_{00}$  does not lead to time-dependent signals to first

order in  $\beta_\oplus$  or  $\beta_L$ ) can be expected, at or below about a part in  $10^{15}$  for the dominating parameters and to about a part in  $10^{11}$  for the parameters that are suppressed by  $\beta_\oplus$ . Future space experiments, for which a resolution of the frequency measurement of up to  $10^{-18}$  is projected [20, 21], might bound the dominating components of  $E'_{jk}$  at the  $10^{-18}$  level, and the suppressed components of  $c_{\mu\nu}$  at the  $10^{-14}$  level.

Instead of using different cavity materials, two cavities made from the same crystalline material, but having different orientations of the cavities with respect to the crystal axes might be used. Using, e.g., quartz, a comparison between a cavity fabricated such that the cavity axis is parallel to the crystals  $c$  axis to one having its cavity axis perpendicular to the  $c$  axis would provide a relatively high sensitivity given by  $\mathcal{B}_{1\Xi}^q$  and  $\mathcal{B}_{3\Xi}^q$ . Another possibility would be two orthogonal cavities within a single block of crystalline material. Such an arrangement might be favourable for eliminating parasitic effects, like thermal expansion and vibration. However, in such an experiment the frequency change  $\delta_{EM}\nu$  due to Lorentz violation in electrodynamics would not drop out, thus complicating the analysis. Another configuration would be the comparison of a cavity against an atomic clock, such as a cesium clock and/or a hydrogen maser. This scenario is interesting, since it is projected for the OPTIS satellite [21]. This satellite is projected to carry three cavities orthogonal to each other, so it is probably possible to separate the electrodynamic terms from the electronic ones in an analysis of the complete data, that consists of all frequency differences between the three cavities and the atomic clock(s). Such an analysis would also have to take into account a possible Lorentz-violating shift of the atomic clock frequencies, which could give the experiment sensitivity to additional parameters.

## VI. SUMMARY AND OUTLOOK

We have calculated the change of the geometry of crystals that is caused by Lorentz invariance violation in the fermionic sector of the extended standard model. The length change is caused by a modified kinetic energy term  $(\delta_{jk} + 2E'_{jk})(1/2m)p_j p_k$  that enters the kinetic energy term of the Hamiltonian for the free electron.  $E'_{jk} = -c_{jk} - \frac{1}{2}c_{00}\delta_{jk}$ , where  $c_{\mu\nu}$  is a Lorentz tensor originating from the standard model extension. The calculation proceeds using a Bloch ansatz for the wave function of the valence electrons with the lattice periodic function given by a Fourier series. The crystal adjusts its geometry such as to minimize its total energy. In that way, Lorentz violation in the electrons' equation of motion affects the length of an electromagnetic cavity that is made from the crystal, and thus the resonance frequency of a cavity made from the material. As a main result of this paper, there is thus a method to measure the  $c_{\mu\nu}$  in cavity tests of Lorentz violation.

Comparing cavities made from different materials, it

is possible to separate the effect connected to  $c_{\mu\nu}$  from Lorentz violation in electrodynamics, that also affects the resonance frequency of cavities. Under some assumptions that help to separate the electrodynamic and the electronic terms, already performed experiments [9, 14, 15] imply constraints on  $c_{XY}$  and  $c_{XX} - c_{YY}$  at the  $10^{-14}$  level, and on  $c_{XX} + c_{YY} - 2c_{ZZ}$  at the  $10^{-12}$  level. This is to our knowledge the only present experimental constraint on the components of  $c_{\mu\nu}$ . We discuss possible setups for experiments that can obtain separate bounds without using these assumptions, and obtain results on more components of  $c_{\mu\nu}$ . Future experiments on Earth and in space promise increased sensitivity up to a part in  $10^{18}$ .

In the appendix, we briefly discuss the case of spin-polarized matter. An additional contribution to the length change arises from a spin-dependent term  $F'_{jkl} \frac{1}{m} p_j p_k \sigma^l$  also originating from the standard model extension. This allows to deduce limits on  $F'_{jkl}$  from experiments using a spin-polarized cavity material, at least in principle.

Our model of the solid state could be improved by using material specific values for the Fourier coefficients of the single electron wave function. Since our model Fourier coefficients already satisfy the symmetry requirements for a realistic wave function, this might result in relatively minor corrections for the length change. A check (maybe for a simple material), however, might be worthwhile. Most importantly, however, a dedicated experiment will be performed to obtain more complete and / or stronger limits on Lorentz violation in the electrons' equation of motion. Cavities made from crystalline sapphire and fused quartz are ready to be implemented.

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### APPENDIX A: SPIN-POLARIZED MATERIALS

For a spin-polarized material, an additional contribution to the geometry change arises from a spin-dependent term of the non relativistic single-electron hamiltonian of the SME, Eq. (3), that is given by  $F'_{jkl}$ . That means, from experiments using cavities made from spin-polarized materials, a limit on  $F'_{jkl}$  can, at least in principle, be deduced. This is interesting, since many degrees of freedom of  $F'_{jkl}$  are not yet fixed experimentally. In this appendix, we estimate the effect and the level of sensitivity that can be expected for such an experiment.

### 1. Hamiltonian

If the average of the spin expectation values is non-zero, the spin-dependent terms contribute to the Lorentz-violating correction to the hamiltonian. We still assume a vanishing average helicity, Eq. (22), for all electrons. Thus,

$$\begin{aligned} \langle \delta h \rangle = & mc^2 B'_j \sum_{a=1}^N \langle (\sigma_a)^j \rangle + \frac{1}{m} E'_{ij} \sum_{a=1}^N \langle (p_a)_i (p_a)_j \rangle \\ & + \frac{1}{m} F'_{jkl} \sum_{a=1}^N \langle (p_a)_j (p_a)_k (\sigma_a)^l \rangle. \end{aligned} \quad (\text{A1})$$

We assume that a fraction  $\eta^i$  of the total  $N$  electrons have their spin  $\frac{1}{2}$  polarized parallel to  $x^i$ . The other electrons are assumed to be unpolarized. The average of the spin expectation values is then given by

$$S^l \equiv \frac{1}{N} \sum_a \langle (\sigma_a)^l \rangle = \frac{1}{2} \eta^l. \quad (\text{A2})$$

For the last term of Eq. (A1),

$$\sum_{a=1}^N \langle (p_a)_j (p_a)_k (\sigma_a)^l \rangle = \frac{1}{2} \eta^l \sum_{a=1}^N \langle (p_a)_j (p_a)_k \rangle. \quad (\text{A3})$$

Therefore,

$$\begin{aligned} \langle \delta h \rangle = & mc^2 \frac{N}{2} B'_j \eta^j \\ & + \frac{1}{m} \left( E'_{ij} + \frac{1}{2} F'_{ijk} \eta^k \right) \sum_{a=1}^N \langle (p_a)_i (p_a)_j \rangle. \end{aligned} \quad (\text{A4})$$

### 2. Geometry change

The term  $mc^2 N B'_j \eta^j / 2$  contained in the hamiltonian is independent from the crystal geometry and does, therefore, not lead to a geometry change. The second term that is proportional to the average of  $\langle p_i p_j \rangle$  over all electrons, however, leads to a geometry change, that can be calculated in analogy to the discussion in the main parts of this paper. We can overtake the result, Eq. (69), for the geometry change if we replace  $E'_{ij}$  by  $\tilde{E}'_{ij} = E'_{ij} + \frac{1}{2} F'_{ijk} \eta^k$ .

The sensitivity of the cavity geometry to  $F'_{jkl}$  is thus given by  $\mathcal{B}_{\Gamma\Xi}$  as well as  $\eta^k$ . The magnitude of the latter can be estimated as the ratio of the number of spin-polarized electrons  $n_{B,u}$  to the total number of electrons  $N_{e,u}$  per unit cell,  $|\eta| = n_{B,u} / n_{e,u}$ . In a saturated ferromagnetic material, e.g. iron at a magnetic field of 1.7 T,  $n_{B,u} \approx 2.2$  [42] spins are polarized per unit cell, so  $|\eta|$  is of order unity. (Note that  $n_{B,u}$  can be as high as  $\simeq 10$  for Dysprosium.) Therefore, the sensitivity of the cavity length (and thus, its resonance frequency) to  $F'_{jkl}$  is comparable to the sensitivity to  $E'_{jk}$ .

### 3. Possible experiments

If the cavity is made from a spin-polarized solid, i.e., a magnetized ferromagnetic material, the cavity length would depend on  $E'_{ij} + F'_{ijk}\eta^k/2$ . That means, from a measurement of the resonance frequency of such a cavity, a limit on  $F'_{ijk}$  could be derived, provided that separate limits on  $E'_{ij}$  are known from previous experiments using one of the methods discussed above. However, note that the systematics of such an experiment are largely unknown. The selection of materials suitable for building stable cavities is a highly nontrivial discussion of the experimental systematics, some of which are far from obvious. Because of the manifold effects connected to magnetization (e.g., magnetostriction), an experiment using a magnetized cavity could suffer from various systematic effects, so our discussion is a bit speculative. A theoretical complication is that practical ferromagnetic materials are usually alloys (such as AlNiCo), whereas the theory presented above is directly applicable for crystals only.

For such a measurement of  $F'_{ijk}$ , one could use a cavity made from a permanent magnetic material. The direction of the spin polarization with respect to the cavity axis determines the components of  $F'_{ijk}$  which dominate the experiment. A rotation of the cavity would modulate the  $F'_{ijk}$ -induced frequency shift. The corresponding time dependency of the cavity resonance frequency would be the signal for a non-zero  $F'_{ijk}$ . It could be beneficial to use solely the Earth's rotation to avoid possible systematics associated with a magnetized cavity rotating in the Earth's magnetic field. Magnetic shielding will probably also be necessary. If the frequency stability of a cavity made from a suitable magnetized material would be of the same order as the stability achieved with quartz or sapphire cavities, limits on  $F'_{ijk}$  of order  $10^{-15}$  could be achieved.

### APPENDIX B: NOTATION CONVENTION IN ELASTICITY THEORY

For obtaining the material specific values of the sensitivity tensor  $\mathcal{B}_{abcd}$ , the compliance tensor  $\mu_{abcd}$  has to be known. The relation between stress  $\sigma_{ij}$  and strain  $e_{dc}$  is given as

$$\sigma_{ij} = \lambda_{ijkl} e_{kl}. \quad (\text{B1})$$

In engineering, it is common to replace this by a six-dimensional matrix equation

$$\sigma = \mathbf{S} \cdot \mathbf{e}, \quad (\text{B2})$$

where [34], p.445

$$\sigma = (\sigma_{xx}, \sigma_{yy}, \sigma_{zz}, \sigma_{yz}, \sigma_{zx}, \sigma_{xy}), \quad (\text{B3})$$

$$\mathbf{e} = (e_{xx}, e_{yy}, e_{zz}, 2e_{yz}, 2e_{zx}, 2e_{xy}), \quad (\text{B4})$$

and

$$\mathbf{S} = \begin{pmatrix} \lambda_{1111} & \lambda_{1122} & \lambda_{1133} & \lambda_{1123} & \lambda_{1131} & \lambda_{1112} \\ \lambda_{2211} & \lambda_{2222} & \lambda_{2233} & \lambda_{2223} & \lambda_{2231} & \lambda_{2212} \\ \lambda_{3311} & \lambda_{3322} & \lambda_{3333} & \lambda_{3323} & \lambda_{3331} & \lambda_{3312} \\ \lambda_{3211} & \lambda_{3222} & \lambda_{3233} & \lambda_{3223} & \lambda_{3231} & \lambda_{3212} \\ \lambda_{3111} & \lambda_{3122} & \lambda_{3133} & \lambda_{3123} & \lambda_{3131} & \lambda_{3112} \\ \lambda_{1211} & \lambda_{1222} & \lambda_{1233} & \lambda_{1223} & \lambda_{1231} & \lambda_{1212} \end{pmatrix}. \quad (\text{B5})$$

This is called the Voigt convention in the literature [37], pp. 604-609. The matrix  $\mathbf{S}$  is symmetric, it thus contains at most 21 independent elements. The symmetry of the crystal reduces the number of independent elements. For example, the matrix for cubic symmetry has three independent elements:

$$\mathbf{S} = \begin{pmatrix} S_{11} & S_{12} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{11} & S_{12} & 0 & 0 & 0 \\ S_{12} & S_{12} & S_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & S_{44} \end{pmatrix}. \quad (\text{B6})$$

For trigonal symmetry, there are six:

$$\mathbf{S} = \begin{pmatrix} S_{11} & S_{12} & S_{13} & S_{14} & 0 & 0 \\ S_{12} & S_{11} & S_{13} & -S_{14} & 0 & 0 \\ S_{13} & S_{13} & S_{33} & 0 & 0 & 0 \\ S_{14} & -S_{14} & 0 & S_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & S_{44} & S_{14} \\ 0 & 0 & 0 & 0 & S_{14} & S_{66} \end{pmatrix} \quad (\text{B7})$$

where

$$S_{66} = 2(S_{11} - S_{12}). \quad (\text{B8})$$

By inverting  $\mathbf{S}$  one obtains the compliance matrix  $\mathbf{C}$  that satisfies  $\mathbf{S} \cdot \mathbf{C} = \mathbf{1}$ , where  $\mathbf{1}$  is the six dimensional unit matrix.  $\mathbf{C}$  enters the equation  $\mathbf{e} = \mathbf{C} \cdot \sigma$  between the stress and strain 6-vectors Eqs. (B3,B4). On the other hand, the compliance *tensor*  $\mu_{abcd}$  enters the relationship between the stress and strain *tensors*,  $e_{ab} = \mu_{abcd}\sigma_{cd}$ . Therefore, the compliance tensor is related to the compliance matrix by

$$\mathbf{C} = \begin{pmatrix} \mu_{1111} & \mu_{1122} & \mu_{1133} & 2\mu_{1123} & 2\mu_{1131} & 2\mu_{1112} \\ \mu_{2211} & \mu_{2222} & \mu_{2233} & 2\mu_{2223} & 2\mu_{2231} & 2\mu_{2212} \\ \mu_{3311} & \mu_{3322} & \mu_{3333} & 2\mu_{3323} & 2\mu_{3331} & 2\mu_{3312} \\ 2\mu_{3211} & 2\mu_{3222} & 2\mu_{3233} & 4\mu_{3223} & 4\mu_{3231} & 4\mu_{3212} \\ 2\mu_{3111} & 2\mu_{3122} & 2\mu_{3133} & 4\mu_{3123} & 4\mu_{3131} & 4\mu_{3112} \\ 2\mu_{1211} & 2\mu_{1222} & 2\mu_{1233} & 4\mu_{1223} & 4\mu_{1231} & 4\mu_{1212} \end{pmatrix}. \quad (\text{B9})$$

The compliance and elasticity matrices for cubical crystals have the same symmetry; for trigonal crystals, the symmetry of the compliance matrix is similar to the one of the elasticity matrix, with the exception that

$C_{66} = \frac{1}{2}(C_{11} - C_{12})$ . The compliance tensor elements  $\mu_{abcd}$  are obtained from the tabulated elements of the elasticity matrix  $\mathbf{S}$  by inverting the elasticity matrix and reading of the tensor elements from Eq. (B9).

### APPENDIX C: SIGNAL COMPONENTS FOR LABORATORY EXPERIMENTS WITH TURNTABLE

Here, we give the full signal components caused by Lorentz violation in the electrons' equation of motion in the laboratory frame for a cavity rotated, using a turntable, at an angular frequency  $\omega_t$ , assuming a material of trigonal or higher crystal symmetry, i.e., the sensitivity matrix  $\mathcal{B}$  is of the form Eq. (82) or simpler. The rotation axis is fixed to point vertically. We use a turntable time scale  $t_t$  defined such that  $t_t = 0$  at any one instant when the cavity is pointing in the  $x$  direction of the laboratory frame.

We use two reference frames, one sun-centered celestial equatorial reference frame and one laboratory frame. As defined in [23], the sun-centered frame has the  $X$  axis pointing towards the vernal equinox (spring point) at 0h right ascension and  $0^\circ$  declination, the  $Z$  axis pointing towards the celestial north pole ( $90^\circ$  declination) and the  $Y$  axis such as to complete the right handed orthogonal dreibein. Earth's equatorial plane lies in the  $X-Y$  plane; its orbital plane is tilted by  $\eta \simeq 23^\circ$  with respect to the latter. The time scale  $T = 0$  when the sun passes the spring point, e.g., on march 20, 2001 at 13:31 UT.

The laboratory frame has the  $x$  axis pointing south, the  $y$  axis east, and the  $z$  axis vertically upwards. The laboratory time scale  $T_\oplus = 0$  when the  $y$  and the  $Y$  axis coincide.

The signal derivation starts from the symmetrized tensor  $c_{(\mu\nu)}$  given in the sun-centered celestial equatorial reference frame, which is suitable for expressing the tensor because it is inertial on all time-scales involved in terrestrial experiments. To  $c_{(\mu\nu)}$ , we first apply a Lorentz boost to first order in  $\beta_\oplus \simeq 10^{-4}$ , the velocity of Earth's orbit

$$\vec{\beta}_\oplus = \beta_\oplus \begin{pmatrix} \sin \Omega_\oplus T \\ -\cos \eta \cos \Omega_\oplus T \\ -\sin \eta \cos \Omega_\oplus T \end{pmatrix}, \quad (\text{C1})$$

where  $\Omega_\oplus \simeq 2\pi/1 \text{ yr}$  is the angular frequency of Earth's orbit. We neglect the smaller velocity  $0 < \beta_L \lesssim 1.5 \times 10^{-6}$  due to Earth's rotation in order not to complicate the signal components below further. Subsequently, application of the rotation matrix

$$R = \begin{pmatrix} \cos \chi \cos \omega_\oplus T_\oplus & \cos \chi \sin \omega_\oplus T_\oplus & -\sin \chi \\ -\sin \omega_\oplus T_\oplus & \cos \omega_\oplus T_\oplus & 0 \\ \sin \chi \cos \omega_\oplus T_\oplus & \sin \chi \sin \omega_\oplus T_\oplus & \cos \chi \end{pmatrix}, \quad (\text{C2})$$

where  $\chi$  is the geographical colatitude, and  $\omega_\oplus \simeq 2\pi/23 \text{ h } 56 \text{ min}$  Earth's rotation angular frequency, leads to the tensor  $c_{\mu\nu}$  as expressed within the laboratory frame. Another rotation around the  $z$  axis using the rotation matrix

$$R_t = \begin{pmatrix} \cos \omega_t t_t & \sin \omega_t t_t & 0 \\ -\sin \omega_t t_t & \cos \omega_t t_t & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (\text{C3})$$

leads to the quantities within the rotating turntable frame, which are then decomposed according to Eq. (8). The time scale  $t_t = 0$  when the cavity axis is parallel to the  $x$  axis. Insertion of the results into Eq. (74) gives the cavity length change, and thus the frequency change that is given below.

For compact notation, we define the abbreviations

$$\omega(a, b, c) = a\omega_t + b\omega_\oplus + c\Omega_\oplus, \quad (\text{C4})$$

$$\phi(a, b, c) = a\omega_t t_t + b\omega_\oplus T_\oplus + c\Omega_\oplus T. \quad (\text{C5})$$

We give the signal components for the two most interesting cavity constructions: A cavity with the resonator axis pointing parallel to the crystals's  $c$  axis (which is currently the most familiar cavity type), and a cavity with the resonator axis parallel to the crystal's  $a$  or  $b$  axis (which gives sensitivity to the  $c_{(0i)}$  components to first order in  $\beta_\oplus$ , the Earth's orbital velocity). The signals are expressed as a Fourier series

$$\frac{\delta\nu}{\nu} = C(0, 0, 0) + \sum_{a,b,c} [S(a, b, c) \sin \phi(a, b, c) + C(a, b, c) \cos \phi(a, b, c)] \quad (\text{C6})$$

with coefficients  $S(a, b, c)$  and  $C(a, b, c)$ ; the dc component  $C(0, 0, 0)$  is not included in the equations below, as it is not measurable.

#### 1. Cavity axis parallel to $a$ axis

We use the abbreviations  $\mathcal{B}_A = \mathcal{B}_{11} + \mathcal{B}_{12} - 2\mathcal{B}_{13}$  and  $\mathcal{B}_B = \mathcal{B}_{11} - \mathcal{B}_{12}$ . The signal consists of 18 frequencies  $\omega(a, b, c)$  with

$$C(0, 1, 0) = -\mathcal{B}_{Ac(XZ)} \cos \chi \sin \chi,$$

$$S(0, 1, 0) = -\mathcal{B}_{Ac(YZ)} \cos \chi \sin \chi,$$

$$C(0, 2, 0) = -(1/4)\mathcal{B}_A(c_{XX} - c_{YY}) \sin^2 \chi,$$

$$S(0, 2, 0) = -(1/2)\mathcal{B}_{Ac(XY)} \sin^2 \chi,$$

$$C(1, -2, 0) = 2\mathcal{B}_{14}c_{(XY)} \cos \frac{\chi}{2} \sin^3 \frac{\chi}{2},$$

$$S(1, -2, 0) = \mathcal{B}_{14}(c_{XX} - c_{YY}) \cos \frac{\chi}{2} \sin^3 \frac{\chi}{2},$$

$$C(1, -1, -1) = -\mathcal{B}_{14}\beta_\oplus \sin^2 \frac{\chi}{2} \sin \frac{\eta}{2} \left( c_{(TY)} \cos \frac{\eta}{2} + c_{(TZ)} \sin \frac{\eta}{2} \right),$$

$$\begin{aligned}
S(1, -1, -1) &= -\frac{1}{2}\mathcal{B}_{14}\beta_{\oplus}c_{(TX)}\sin^2\frac{\chi}{2}\sin\eta, \\
C(1, -1, 0) &= \mathcal{B}_{14}c_{(YZ)}(1+2\cos\chi)\sin^2\frac{\chi}{2}, \\
S(1, -1, 0) &= \mathcal{B}_{14}c_{(XZ)}(1+2\cos\chi)\sin^2\frac{\chi}{2}, \\
C(1, -1, 1) &= \mathcal{B}_{14}\beta_{\oplus}\cos\frac{\eta}{2}\sin^2\frac{\chi}{2}\left(c_{(TZ)}\cos\frac{\eta}{2}\right. \\
&\quad \left.-c_{(TY)}\sin\frac{\eta}{2}\right), \\
S(1, -1, 1) &= -\frac{1}{2}\mathcal{B}_{14}\beta_{\oplus}c_{(TX)}\sin^2\frac{\chi}{2}\sin\eta, \\
C(1, 0, -1) &= -(1/2)\mathcal{B}_{14}\beta_{\oplus}c_{(TX)}\cos\eta\sin\chi, \\
S(1, 0, -1) &= (1/2)\mathcal{B}_{14}\beta_{\oplus}c_{(TY)}\sin\chi, \\
C(1, 0, 0) &= 0, \\
S(1, 0, 0) &= -(1/4)\mathcal{B}_{14}(c_{XX}+c_{YY}-2c_{ZZ})\sin 2\chi, \\
C(1, 0, 1) &= -(1/2)\mathcal{B}_{14}\beta_{\oplus}c_{(TX)}\cos\eta\sin\chi, \\
S(1, 0, 1) &= -(1/2)\mathcal{B}_{14}\beta_{\oplus}c_{(TY)}\sin\chi, \\
C(1, 1, -1) &= -\mathcal{B}_{14}\beta_{\oplus}\cos^2\frac{\chi}{2}\cos\frac{\eta}{2}\left(c_{(TZ)}\cos\frac{\eta}{2}\right. \\
&\quad \left.-c_{(TY)}\sin\frac{\eta}{2}\right), \\
S(1, 1, -1) &= -\frac{1}{2}\mathcal{B}_{14}\beta_{\oplus}c_{(TX)}\cos^2\frac{\chi}{2}\sin\eta, \\
C(1, 1, 0) &= \mathcal{B}_{14}c_{(YZ)}\cos^2\frac{\chi}{2}(2\cos\chi-1), \\
S(1, 1, 0) &= -\mathcal{B}_{14}c_{(XZ)}\cos^2\frac{\chi}{2}(2\cos\chi-1), \\
C(1, 1, 1) &= \mathcal{B}_{14}\beta_{\oplus}\cos^2\frac{\chi}{2}\sin\frac{\eta}{2}\left(c_{(TY)}\cos\frac{\eta}{2}\right. \\
&\quad \left.+c_{(TZ)}\sin\frac{\eta}{2}\right), \\
S(1, 1, 1) &= -\frac{1}{2}\mathcal{B}_{14}\beta_{\oplus}c_{(TX)}\cos^2\frac{\chi}{2}\sin\eta, \\
C(1, 2, 0) &= (1/2)\mathcal{B}_{14}c_{(XY)}(1+\cos\chi)\sin\chi, \\
S(1, 2, 0) &= -\mathcal{B}_{14}(c_{XX}-c_{YY})\cos^3\frac{\chi}{2}\sin\frac{\chi}{2}, \\
C(2, -2, 0) &= \frac{1}{2}\mathcal{B}_B(c_{XX}-c_{YY})\sin^4\frac{\chi}{2}, \\
S(2, -2, 0) &= -\mathcal{B}_Bc_{(XY)}\sin^4\frac{\chi}{2}, \\
C(2, -1, 0) &= 2\mathcal{B}_Bc_{(XZ)}\cos\frac{\chi}{2}\sin^3\frac{\chi}{2}, \\
S(2, -1, 0) &= -2\mathcal{B}_Bc_{(YZ)}\cos\frac{\chi}{2}\sin^3\frac{\chi}{2}, \\
C(2, 0, 0) &= -(1/4)\mathcal{B}_B(c_{XX}+c_{YY}-2c_{ZZ})\sin^2\chi,
\end{aligned}$$

$$\begin{aligned}
S(2, 0, 0) &= 0, \\
C(2, 1, 0) &= -2\mathcal{B}_Bc_{(XZ)}\cos^3\frac{\chi}{2}\sin\frac{\chi}{2}, \\
S(2, 1, 0) &= -2\mathcal{B}_Bc_{(YZ)}\cos^3\frac{\chi}{2}\sin\frac{\chi}{2}, \\
C(2, 2, 0) &= \frac{1}{2}\mathcal{B}_B(c_{XX}-c_{YY})\cos^4\frac{\chi}{2}, \\
S(2, 2, 0) &= \mathcal{B}_Bc_{(XY)}\cos^4\frac{\chi}{2}.
\end{aligned}$$

The signal for a cavity parallel to the crystals  $b$  axis can be obtained from these equations, if the  $x$  and  $y$  axis are interchanged.

## 2. Signal for a cavity parallel to the $c$ axis

The cavity is oriented with its axis parallel to the  $x_t$  axis. We introduce the abbreviations  $\mathcal{B}_C = -2\mathcal{B}_{31} + \mathcal{B}_{32} + \mathcal{B}_{33}$  and  $\mathcal{B}_D = \mathcal{B}_{32} - \mathcal{B}_{33}$ . (For the trigonal case, Eq. (82),  $\mathcal{B}_{32} = \mathcal{B}_{31}/3$ , for isotropic materials,  $\mathcal{B}_{32} = \mathcal{B}_{31}$ .) We have seven signal frequencies with the amplitudes

$$\begin{aligned}
C(0, 1, 0) &= -\mathcal{B}_Cc_{(XZ)}\cos\chi\sin\chi, \\
S(0, 1, 0) &= -\mathcal{B}_Cc_{(YZ)}\cos\chi\sin\chi, \\
C(0, 2, 0) &= -(1/4)\mathcal{B}_C(c_{XX}-c_{YY})\sin^2\chi, \\
S(0, 2, 0) &= -(1/2)\mathcal{B}_Cc_{(XY)}\sin^2\chi, \\
C(2, -2, 0) &= -\frac{1}{2}\mathcal{B}_D(c_{XX}-c_{YY})\sin^4\frac{\chi}{2}, \\
S(2, -2, 0) &= \mathcal{B}_Dc_{(XY)}\sin^4\frac{\chi}{2}, \\
C(2, -1, 0) &= -2\mathcal{B}_Dc_{(XZ)}\cos\frac{\chi}{2}\sin^3\frac{\chi}{2}, \\
S(2, -1, 0) &= 2\mathcal{B}_Dc_{(YZ)}\cos\frac{\chi}{2}\sin^3\frac{\chi}{2}, \\
C(2, 0, 0) &= (1/4)\mathcal{B}_D(c_{XX}+c_{YY}-2c_{ZZ})\sin^2\chi, \\
S(2, 0, 0) &= 0, \\
C(2, 1, 0) &= 2\mathcal{B}_Dc_{(XZ)}\cos^3\frac{\chi}{2}\sin\frac{\chi}{2}, \\
S(2, 1, 0) &= 2\mathcal{B}_Dc_{(YZ)}\cos^3\frac{\chi}{2}\sin\frac{\chi}{2}, \\
C(2, 2, 0) &= -\frac{1}{2}\mathcal{B}_D(c_{XX}-c_{YY})\cos^4\frac{\chi}{2}, \\
S(2, 2, 0) &= -\mathcal{B}_Dc_{(XY)}\cos^4\frac{\chi}{2}.
\end{aligned}$$

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- $$0 = \sum_a \sum_{\vec{n}} |(c_{\vec{n}})_a|^2 [(q_a)_i + \hbar n_j k_{ij}],$$
- which is derived in analogy to Eq. (26). The quasi-momenta  $q_a$  are within the first Brillouin zone. Thus, as explained after Eq. (28), the two terms cannot cancel each other, so
- $$\sum_a \sum_{\vec{n}} |(c_{\vec{n}})_a|^2 n_j k_{ij} = 0.$$
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