Phenomenological field theories for layered materials: Equations of motion and continuity conditions

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In many cases synthetic structures are specified on length scales large compared to the interatomic distances. On such scales local phenomenological field theories are being used that dispose of the atomic structure but allow one to make extensive use of higher-level bulk properties. We derive equations of motion including higher-order spatial derivatives, which can be adopted to various effective continua like Schrödinger fields for electrons in solids, electromagnetic fields in dielectrics, and acoustic or optical displacement fields. For these generalized fields we solve the long-standing problem of how to derive a complete set of continuity conditions at a plane interface. In the same way continuity conditions for interacting fields (e.g., polaritons) are obtained.

I. INTRODUCTION

In recent years the rapidly developing techniques for creating artificial structures on a submicrometer scale[1] have tended to direct much interest from the ideal homogeneous solid state, the traditional realm of fundamental research, to the understanding of considerably more complex structures, the dynamics of which are basic also to device physics. The design variations of such inhomogeneous systems appear almost indefinite. An important class to be discussed here concerns structural changes in one direction, in particular, layered structures.

In principle, existing theoretical schemes developed for homogeneous systems can be extended to deal with such inhomogeneous materials. As far as phonons are concerned, there are detailed lattice-dynamical studies for slabs,[2] superlattices,[3] and double heterojunctions,[4] and corresponding investigations based on a set of local atomic wave functions for electron states.[5,6] Nevertheless, an alternative though less fundamental approach has been quite successful: In the continuum approximation for displacement fields[7,8] the inhomogeneous structure is described in terms of spatially dependent elastic coefficients. In the same way, the so-called envelope function approximation for electrons[9,10] makes explicit use only of bulk parameters like band edge and effective mass, and a model for their spatial variation. A classical example of renewed interest is continuum electrodynamics[11] with, e.g., spatial variations of the dielectric constant.[12] All these phenomenological structure models thus define phenomenological field theories for the phonon, the electron, and the light field, respectively.

The possibility of such schemes rests upon the existence of different inherent length scales. In simple crystalline materials there is basically one inherent length scale: the typical interatomic distance L_0. Complex structures contain additional (larger) length scales L_i, which may even form a hierarchy, like in superlattices. If $L_i \ll L_{i+1}$ holds, a finite level of resolution Δr with $L_i < \Delta r < L_{i+1}$ will focus on longer-scale patterns, while short-scale modulations (with respect to the structure as well as with respect to the field) are ignored. Any such phenomenological structure model thus defines homogeneity as a scale-dependent concept: What appears as a (periodic) structure on one level is homogeneous on the other.

Despite its obvious limitations phenomenological field theory is able to address most directly two pertinent problems of inhomogeneous systems: How does the parameter field pattern influence the linear modes? And how does it influence the interactions (i.e., mode dynamics)? As input only the local bulk parameters and their spatial dependence are required. For heterojunctions with their discontinuous parameter changes, no additional information about the interface enters (on the accepted level of resolution): This is convenient since such microscopic information is usually very scarce anyway.

In this investigation we apply phenomenological field theory to the phenomenological electromagnetic field, the effective Schrödinger field, and acoustic and optical displacement fields in layered structures. The accepted spatial resolution is $\Delta r \gg L_0$. We briefly discuss approaches with further reduced resolution. This is a generalization of conventional continuum theory in several respects: the systematic account of various fields of different physical origin, the inclusion of dispersive corrections, and the definition of continuity conditions at interfaces.

This paper is organized as follows. In Sec. II we briefly review the connection between static structure fields and dynamical fields as it applies to a treatment of inhomogeneous systems. Continuity conditions are derived from the pertinent balance equations. The electromagnetic field and the phenomenological Schrödinger field are discussed as examples in Secs. III and IV, respectively. We then introduce multiple displacement fields in Sec. V, and in Sec. VI mutual field interactions.

II. PHENOMENOLOGICAL FIELD THEORY

Formal similarities between the Schrödinger field equation, say, and the electromagnetic wave equation, have, of course, long since been noted (see, e.g., Ref. 13). Lagrangians including higher derivatives have been discussed previously (see, e.g., Refs. 14–16). It appears, however, that these analogies and generalizations have not been systematically exploited in the context of inhomogeneous structures defined by parameter fields. We therefore start with a brief review of local-field theory.

A. Local-field approximation picture

Let $\Psi_i(\mathbf{x})$ be an arbitrary vector field on $\mathbf{x}=\{x_0,x_1,x_2,x_3\}=\{t,r_1,r_2,r_3\}$, the dynamics of which is determined by the extremum property of the action functional $S[\Psi_i(\mathbf{x})]=\int dx_0 L$, where L denotes the respective Lagrangian. We assume $S[\Psi_i(\mathbf{x})]$ to have the nonlocal and retarded form

$$S[\Psi_i(\mathbf{x})]=\tfrac{1}{2}\int\int d^4\mathbf{x}\, d^4\mathbf{x}'\tilde{\beta}_{ij}(\mathbf{x},\mathbf{x}')\Psi_i(\mathbf{x})\Psi_j(\mathbf{x}') +\tfrac{1}{6}\int\int\int d^4\mathbf{x}\, d^4\mathbf{x}' d^4\mathbf{x}''\tilde{\gamma}_{ijk}(\mathbf{x},\mathbf{x}',\mathbf{x}'') \times\Psi_i(\mathbf{x})\Psi_j(\mathbf{x}')\Psi_k(\mathbf{x}'')+\cdots . \tag{2.1}$$

Here and below summation is implied for any repeated index in an individual term. We use the convention that indices following a common denote differentiation with respect to this coordinate, e.g., $\Psi_{i,j}=\partial\Psi_i/\partial x_j$, etc. Greek indices are 0,1,2,3; Latin indices will be restricted to 1,2,3 unless stated otherwise. Transforming to Jacobi coordinates (see Ref. 17), e.g., $(\mathbf{x},\mathbf{x}')\rightarrow(\mathbf{x}^s,\xi)$, with

$$\mathbf{x}^s=\tfrac{1}{2}(\mathbf{x}+\mathbf{x}'),\quad \xi=\mathbf{x}-\mathbf{x}' , \tag{2.2}$$

(2.1) can be written as

$$S[\Psi_i(\mathbf{x})]=\int d^4\mathbf{x}^s\left[\int d^4\xi\left[\frac{J_1}{2}\beta_{ij}(\mathbf{x}^s,\xi)\Psi_i(\mathbf{x}^s+\tfrac{1}{2}\xi)\Psi_j(\mathbf{x}^s-\tfrac{1}{2}\xi) +\int d^4\eta\frac{J_2}{6}\gamma_{ijk}(\mathbf{x}^s,\xi,\eta)\Psi_i(\mathbf{x}^s+\tfrac{1}{2}\xi-\tfrac{1}{3}\eta)\Psi_j(\mathbf{x}^s-\tfrac{1}{2}\xi-\tfrac{1}{3}\eta)\Psi_k(\mathbf{x}^2+\tfrac{2}{3}\eta)+\cdots\right]\right] . \tag{2.3}$$

The J_i are the respective Jacobi determinants, and since the transformation preserves volume and direction, $J_i=1$ holds. The integrand in the outer brackets is the Lagrangian density $\mathcal{L}(x^s)$.

We will presently consider only the bilinear term in (2.3), keeping in mind that multilinear terms of higher order appear, e.g., in Coulomb interaction or lattice anharmonicity. The Lagrangian density reads

$$\mathcal{L}(x^s)=\tfrac{1}{2}\int d^4\xi\,\beta_{ij}(\mathbf{x}^s,\xi)\Psi_i(\mathbf{x}^s+\tfrac{1}{2}\xi)\Psi_j(\mathbf{x}^s-\tfrac{1}{2}\xi) , \tag{2.4}$$

To derive the equation of motion we should have more information about the kernel β in (2.4). Let us assume that β_{ij} decreases exponentially with $|\xi|$ on a scale on which the field changes are small compared to this. We are then allowed to expand the field product into a Taylor series around $\mathbf{x}^s$ implying

$$2\mathcal{L}(\mathbf{x}^s)=\int d^4\xi\,\beta_{ij}(\mathbf{x}^s,\xi)\mathcal{D}\Psi_i(\mathbf{x})\Psi_j(\mathbf{x}')\big|_{\mathbf{x},\mathbf{x}'=\mathbf{x}^s} \tag{2.5}$$

with the operator

$$\mathcal{D}=\left[1+\left[\frac{\xi_\nu}{2}\right]\frac{\partial}{\partial x_\nu}+\left[\frac{-\xi_{\nu'}}{2}\right]\frac{\partial}{\partial x'_{\nu'}} +\frac{1}{2}\left[\frac{\xi_\mu}{2}\right]\left[\frac{\xi_\nu}{2}\right]\frac{\partial^2}{\partial x_\mu\partial x_\nu} +\frac{1}{2}\left[\frac{\xi_\nu}{2}\right]\left[\frac{-\xi_{\nu'}}{2}\right]\frac{\partial^2}{\partial x_\nu\partial x'_{\nu'}}+\cdots\right] . \tag{2.6}$$

We thus find, comprising all terms involving time derivatives into $\mathcal{L}_0$,

$$2\mathcal{L}=2\mathcal{L}_0-B_{ii'}\Psi_i\Psi_{i'}-C_{ij|i'}\Psi_{i,j}\Psi_{i'}-C_{i|i'j'}\Psi_i\Psi_{i',j'} -D_{ij|i'j'}\Psi_{i,j}\Psi_{i',j'}-D_{ijk|i'}\Psi_{i,jk}\Psi_{i'} -D_{i|i'j'k'}\Psi_i\Psi_{i',j'k'}-\cdots \tag{2.7}$$

with the coupling tensors (signs chosen to have the "potential energy" positive, see applications below)

$$\begin{aligned} B_{ii'}(\mathbf{x}^s)&=-\int d^4\xi\,\beta_{ii'}(\mathbf{x}^s,\xi)=B_{i'i}(\mathbf{x}^s) ,\\ C_{ij|i'}(\mathbf{x}^s)&=-\tfrac{1}{2}\int d^4\xi\,\beta_{ii'}(\mathbf{x}^s,\xi)\xi_j=-C_{i|i'j}(\mathbf{x}^s) ,\\ D_{ij|i'j'}(\mathbf{x}^s)&=-\tfrac{1}{8}\int d^4\xi\,\beta_{ii'}(\mathbf{x}^s,\xi)\xi_j(-\xi_{j'})\\ &=-D_{i|i'j'j}(\mathbf{x}^s) , \end{aligned} \tag{2.8}$$

etc. In this integral representation the coupling tensors appear as moments of ξ_j over the "weight function" $\beta_{ii'}$ (cf. Mills[18] for a similar representation of the dielectric tensor). The relations between the various coupling tensors as expressed in (2.8) also follow directly from (2.7) by partial integration (plus appropriate boundary conditions). Alternatively we may write (2.7) as

$$2\mathcal{L}=2\mathcal{L}_0+\frac{\partial^2\mathcal{L}}{\partial\Psi_i\partial\Psi_{i'}}\bigg|_0\Psi_i\Psi_{i'}+2\frac{\partial^2\mathcal{L}}{\partial\Psi_{i,j}\partial\Psi_{i'}}\bigg|_0\Psi_{i,j}\Psi_{i'} +2\frac{\partial^2\mathcal{L}}{\partial\Psi_i\partial\Psi_{i',j'}}\bigg|_0\Psi_i\Psi_{i',j'}+\frac{\partial^2\mathcal{L}}{\partial\Psi_{i,j}\partial\Psi_{i',j'}}\bigg|_0\Psi_{i,j}\Psi_{i',j'} +2\frac{\partial^2\mathcal{L}}{\partial\Psi_{i,jk}\partial\Psi_{i'}}\bigg|_0\Psi_{i,jk}\Psi_{i'}+2\frac{\partial^2\mathcal{L}}{\partial\Psi_i\partial\Psi_{i',j'k'}}\bigg|_0\Psi_i\Psi_{i',j'k'} , \tag{2.9}$$

where all the second-order field derivatives of $\mathcal{L}$ have to be taken at $\Psi_i=0$, $\Psi_{i,j}=0$, etc. These give, by comparison with (2.7), another interpretation of the coupling tensors (2.8).

For field equations of second order in time we require

$$2\mathcal{L}_0=B^0_{ii'}\dot{\Psi}_i\dot{\Psi}_{i'} \tag{2.10}$$

with $\dot{\Psi}_i=\Psi_{i,0}$ and the second-rank parameter tensor

$$B^0_{ii'}=\left.\frac{\partial^2\mathcal{L}}{\partial\dot{\Psi}_i\partial\dot{\Psi}_{i'}}\right|_0=\tfrac{1}{8}\int d^4\xi\,\beta_{ii'}(\mathbf{x}^s,\xi)\xi_0(-\xi_0)\ , \tag{2.11}$$

so that $\mathcal{L}=\mathcal{L}(\Psi_i,\dot{\Psi}_i,\Psi_{i,j},\Psi_{i,jk},\ldots,x^s_\mu)$, i.e., only spatial derivatives of finite order are supposed to appear. The equation of motion for the dynamical field Ψ_i reads for[19] (2.7)

$$-\frac{\partial\mathcal{L}}{\partial\Psi_i}+\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{\Psi}_i}+\frac{d}{dr_j}\left[\frac{\partial\mathcal{L}}{\partial\Psi_{i,j}}\right]-\frac{d^2}{dr_jdr_k}\left[\frac{\partial\mathcal{L}}{\partial\Psi_{i,jk}}\right]+\cdots=0\ . \tag{2.12}$$

One is easily convinced that, e.g.,

$$\mathcal{L}=\mathcal{L}_0+D_{ij|i'j'}\Psi_{i,j}\Psi_{i',j'} \tag{2.13}$$

and

$$\mathcal{L}'=\mathcal{L}_0-D_{ij|i'j'}\Psi_i\Psi_{i',j'j}=\mathcal{L}_0+D_{i|i'j'j}\Psi_i\Psi_{i',j'j} \tag{2.14}$$

(which differ by a divergence) produce the same equation of motion. This (well-known) nonuniqueness of $\mathcal{L}$ can be reduced by considering certain standard forms, e.g., the symmetric (2.13) instead of (2.14). This will typically be the case for the applications in the following sections.

The conjugate field to $\dot{\Psi}_i$ is the canonical momentum density

$$\pi_i=\frac{\partial\mathcal{L}}{\partial\dot{\Psi}_i}\ , \tag{2.15}$$

which, if $\dot{\Psi}_i=\dot{\Psi}_i(\pi_j,\Psi_j,\Psi_{j,k},\ldots)$ exists, allows one to introduce the Hamiltonian density by $\mathcal{H}=\dot{\Psi}_i\pi_i-\mathcal{L}$. Field quantization is obtained, as usual, by taking Poisson brackets into commutators, so that the classical field equations become the operator equations of the Heisenberg picture.

If $\mathcal{L}$ does not explicitly depend on $\mathbf{x}^s$, we have a conservative homogeneous system, for which all parameters are constant. Any explicit spatial dependence of $\mathcal{L}$ must necessarily be represented by the expansion coefficients (2.8). Inhomogeneity therefore leads to the concept of parameter fields: Their pattern constitutes a phenomenological structure model of given spatial resolution to which the dynamical properties must be referred. If one accepts that phenomenological field theories also should be of Lagrangian type, the separation of any Lagrange term into a contraction of a tensorial parameter and field derivatives is uniquely defined: There can be no dispute about what to consider as the proper parameter field and the equations of motion are unambiguously specified.[20] The nature of the parameters, to be sure, depends on the level of description. They are constrained by point symmetry and other model-dependent restrictions. Parameter fields give rise to modified equations of motion.

B. Balance equations

Equation (2.12) can be written as a balance equation for the conjugate field π_i:

$$\dot{\pi}_i+\frac{d}{dr_j}p_{ij}=\frac{\partial\mathcal{L}}{\partial\Psi_i}\ , \tag{2.16}$$

where p_{ij} is the (conjugate) momentum current tensor

$$p_{ij}=\frac{\partial\mathcal{L}}{\partial\Psi_{i,j}}-\frac{d}{dr_k}\frac{\partial\mathcal{L}}{\partial\Psi_{i,jk}}+\frac{d}{dr_k}\frac{d}{dr_m}\frac{\partial\mathcal{L}}{\partial\Psi_{i,jkm}}-\cdots\ . \tag{2.17}$$

The right-hand side of Eq. (2.16) disappears, if Ψ_i is a cyclic field variable. In general, p_{ij} is not necessarily symmetric.

We note that this balance equation (2.16) can be recast into the recursive form

$$\frac{d}{dr_j}a_i^j=\frac{\partial\mathcal{L}}{\partial\Psi_i}-\frac{d}{dt}\frac{\partial\mathcal{L}}{\partial\dot{\Psi}_i} \tag{2.18}$$

with

$$\begin{aligned}a_i^j&=\frac{\partial\mathcal{L}}{\partial\Psi_{i,j}}-\frac{d}{dr_k}b_i^{jk}\ ,\\ b_i^{jk}&=\frac{\partial\mathcal{L}}{\partial\Psi_{i,jk}}-\frac{d}{dr_l}c_i^{jkl}\ ,\\ c_i^{jkl}&=\frac{\partial\mathcal{L}}{\partial\Psi_{i,jkl}}-\cdots\ .\end{aligned} \tag{2.19}$$

For the energy momentum balance we obtain as usual

$$\frac{d}{dx_\mu}\Theta_{\mu\nu}=\left[\frac{\partial\mathcal{L}}{\partial x_\nu}\right]_{\text{ex}}\ ,\quad \nu=0,1,2,3 \tag{2.20}$$

where $(\partial\mathcal{L}/\partial x_\mu)_{\text{ex}}$ denotes the explicit derivative of $\mathcal{L}$ with respect to the variable x_μ, and the (nonsymmetric) energy-momentum tensor is

$$\Theta_{\mu\nu}=\mathcal{L}\delta_{\mu\nu}-a_i^\mu\Psi_{i,\nu}-b_i^{\mu\lambda}\Psi_{i,\lambda\nu}-c_i^{\mu\lambda\gamma}\Psi_{i,\lambda\gamma\nu}\cdots\ . \tag{2.21}$$

For the Lagrangian (2.7) with (2.10), the terms of (2.19) involving the time derivative are

$$\begin{aligned}a_i^0&=\frac{\partial\mathcal{L}}{\partial\dot{\Psi}_i}=\pi_i\ ,\\ b_i^{\mu\lambda}&=0\quad\text{for }\mu\nu=0\end{aligned} \tag{2.22}$$

etc. For $\nu=0$ (2.20) represents the local energy balance equation

$$\frac{\partial}{\partial t}\mathcal{H}+\operatorname{div}\mathbf{S}=\left[\frac{\partial\mathcal{L}}{\partial t}\right]_{\text{ex}}=0\ , \tag{2.23}$$

where the energy density has been identified as

$$\Theta_{00}=\pi_i\dot{\Psi}_i-\mathcal{L}=\mathcal{H} \tag{2.24}$$

and the energy current density as

$$S_j=\Theta_{j0}=-a_i^j\dot{\Psi}_i-b_i^{jk}\dot{\Psi}_{i,k}-c_i^{jkl}\dot{\Psi}_{i,kl}\cdots \quad (2.25)$$

We note that S_j decomposes into exactly γ terms if γ is the highest-order spatial derivative appearing in $\mathcal{L}$ [cf. (2.19)]. If $\mathcal{L}$ includes this highest derivative in bilinear form, the highest-order spatial derivative in the equation of motion (2.18) is 2γ. For $j=1,2,3$ we obtain the momentum balance

$$\frac{\partial}{\partial t}q_j+\frac{\partial}{\partial r_i}P_{ij}=\left[\frac{\partial\mathcal{L}}{\partial r_j}\right]_{\text{ex}}, \quad (2.26)$$

where the (translational) momentum density is

$$q_j=\Theta_{0j}=-\pi_i\Psi_{i,j} \quad (2.27)$$

and the momentum current density

$$P_{ij}=\mathcal{L}\delta_{ij}-a_k^i\Psi_{k,j}-b_k^{il}\Psi_{k,lj}-c_k^{ilm}\Psi_{k,lmj}-\cdots \quad (2.28)$$

As is well known, this tensor is not uniquely defined: it can be symmetrized to satisfy the balance of angular momentum. For a homogeneous system momentum is conserved, as $(\partial\mathcal{L}/\partial r_i)_{\text{ex}}=0$; for one-dimensional inhomogeneity, where $\mathcal{L}$ depends explicitly on r_3 only, $(\partial\mathcal{L}/\partial r_3)_{\text{ex}}\neq 0$ acts as a source term for q_3.

C. Layered structures: Bulk-mode representation

1. *Constrained superpositions*

If $\mathcal{L}$ does not depend explicitly on r_i, all the phenomenological parameters are constant, and the respective equation of motion is solved by plane wave (e.g., for periodic boundary conditions). Due to the linearity any solution can be written as a superposition of such modes. Special superpositions are required by additional constraints: The origin of these may be traced back to additional continuity conditions at interfaces and/or preparation.

For layered structures the individual bulk mode, in general, no longer satisfies those continuity conditions, so that specific superpositions (including nonpropagating modes, e.g., complex k_i) will have to be considered in any sublayer. A layered structure as a one-dimensional inhomogeneous system violates translational invariance only in one direction, say the r_3 direction. According to Bloch's theorem we may thus write (complex representation)

$$\Psi_j(\mathbf{r},t)=e_je^{i(\mathbf{k}_\parallel\mathbf{R}-\omega t)}\varphi(r_3) \quad (2.29)$$

with $\mathbf{k}_\parallel=(k_1,k_2)$ being real and $\mathbf{R}=(r_1,r_2)$. $\mathbf{e}$ is the polarization vector, $|\mathbf{e}|=1$. Here we restrict ourselves to a heterojunction, in which a single-plane interface at $r_3=0$ separates medium (1) in $r_3<0$ from medium (2) in $r_3>0$. An eigenmode of this structure may thus be specified by ω and $\mathbf{k}_\parallel$, while $\varphi(r_3)$ can be represented as a superposition of the (in general complex) solutions k_3 of $\omega^2(k_\parallel,k_3)=\omega^2$ in medium (1) and (2), respectively, with, in general, three independent polarization vectors $\mathbf{e}^l$ for each allowed $\mathbf{k}$ (in the case of a three-dimensional vector-field). If $\omega^2(k_\parallel,k_3)=\omega^2$ in medium (i) is of order $N(i)$ in k_3, there are $N(i)$ (in general complex) solutions. We note that if the highest-order field derivative in $\mathcal{L}$ is $\gamma(i)$ and included in bilinear form, we have $N(i)=2\gamma(i)$. Let $N_+(i)$ be the number of real solutions with $k_3>0$, $N_-(i)$ those with $k_3<0$, $K_+(i)$ the number of solutions with $\text{Im}k_3>0$, $K_-(i)$ those with $\text{Im}k_3<0$. Then

$$2\gamma(i)=N_+(i)+N_-(i)+K_+(i)+K_-(i),\quad i=1,2\ . \quad (2.30)$$

It is convenient to further restrict the superposition in medium (1) to one propagating incoming mode of given amplitude $\varphi^0=1$ and polarization e_j^0 together with the $M(1)=N_-(1)+K_-(1)$ modes and the $M(2)=N_+(2)+K_+(2)$ modes in medium (2). [The nonpropagating modes $K_+(2),K_-(1)$ will give rise to localized modes at the interface.] With $N_-(i)+K_-(i)=N_+(i)+K_+(i)$ we obtain

$$M(i)=\gamma(i) \quad (2.31)$$

so that

$$\Psi_j(1)=e^{i(\mathbf{k}_\parallel\mathbf{R}-\omega t)}\times\left\{e_j^0e^{ik_3^0r_3}+\sum_{l=1}^{3}\sum_{m=1}^{\gamma(1)}\varphi^{lm}(1)e_j^{lm}e^{-ik_3^mr_3}\right\},\quad r_3\le 0 \quad (2.32)$$

$$\Psi_j(2)=e^{i(\mathbf{k}_\parallel\mathbf{R}-\omega t)}\sum_{l=1}^{3}\sum_{m=1}^{\gamma(2)}\varphi^{lm}(2)e_j^{lm}e^{ik_3^mr_3},\quad r_3\ge 0\ .$$

It is clear that all these $3[\gamma(1)+\gamma(2)]$ as yet undetermined (in general) complex amplitudes φ^{lm} should result from the same number of continuity conditions. There cannot be any ambiguity as this scenario corresponds to a typical experimental situation for which a unique solution must be expected. However, it is not obvious how these conditions might be found at all. It will be shown that they follow from rather general assumptions about the interface: energy conservation and linearity.

2. *Continuity conditions*

(a) *Energy conservation.* If $(\partial\mathcal{L}/\partial x_\nu)_{\text{ex}}=0$, with $\nu\neq 3$ we obtain, applying Gauss's theorem to (2.20),

$$\Theta_{3\nu}(1)=\Theta_{3\nu}(2)\quad\text{for }\nu\neq 3\ . \quad (2.33)$$

For $\nu=0$ we thus arrive at the continuity condition for the energy current density in the r_3 direction,

$$S_3=-a_i^3\dot{\Psi}_i-b_i^{3j}\dot{\Psi}_{i,j}-c_i^{3jk}\dot{\Psi}_{i,jk}-\cdots, \quad (2.34)$$

while for $\nu=n=1,2$ at the continuity for the momentum current density,

$$\Theta_{3n}=-a_i^3\Psi_{i,n}-b_i^{3j}\Psi_{i,jn}-c_i^{3jk}\Psi_{i,jkn}-\cdots\ . \quad (2.35)$$

Due to translational symmetry in the r_1,r_2 plane we can replace $\partial/\partial r_j$ by ik_j for $j=1,2$ and thus rewrite (2.34)

$$S_3=-A_i\dot{\Psi}_i-B_i\dot{\Psi}_{i,3}-C_i\dot{\Psi}_{i,333}-\cdots, \quad (2.36)$$

where

$$A_i = a_i^3 + i \sum_{j\neq 3} b_i^{3j} k_j - \sum_{j,l\neq 3} c_i^{3jk} k_j k_l + \cdots ,$$
$$B_i = b_i^{33} + 2i \sum_{j\neq 3} c_i^{33j} k_j + \cdots , \tag{2.37}$$
$$C_i = c_i^{333} + \cdots .$$

There are exactly $\gamma(\nu)$ such vectors in medium (ν) not equal to zero (confer the discussion in Sec. II B). For dispersionless field modes we obtain $S_3=0$, and there are no continuity conditions at all. The continuity of Θ_{3n}, $n=1,2$, does not lead to any additional constraint.

(b) *Linearity.* For a linear field we expect that the reflection and transmission patterns of any incoming mode are not changed by the presence of another mode. This means that the continuity conditions must be linear in the field. In order that S_3 is continuous for any superposition of modes, the *individual* factors appearing in (2.36) should be continuous at $r_3=0$. If we restrict ourselves to the case $\gamma(1)=\gamma(2)=\gamma$, this results in 2γ complex vector equations, e.g., for $\gamma=3$:

$$A_i(1)=A_i(2),\quad \Psi_i(1)=\Psi_i(2),\quad i=1,2,3$$
$$B_i(1)=B_i(2),\quad \Psi_{i,3}(1)=\Psi_{i,3}(2) , \tag{2.38}$$
$$C_i(1)=C_i(2),\quad \Psi_{i,33}(1)=\Psi_{i,33}(2) .$$

These conditions must be satisfied by the ansatz (2.32) thus leading to a set of 6γ linear algebraic equations for the 6γ amplitudes $\varphi^{lm}(1),\varphi^{lm}(2)$. If $\gamma(1)>\gamma(2)$, e.g., $\gamma(1)=3,\gamma(2)=2$, the last line of (2.38) would read

$$C_i(1)=0,\quad \Psi_{i,33}(1) \text{ unconstrained} ,$$

which are $3[\gamma(1)+\gamma(2)]$ equations as required.

Under special conditions these equations are solved by real amplitudes φ^{lm}, i.e., without additional phase factors. This is the case if the $A_i,B_i,C_i,\ldots$ contain either odd or even spatial derivatives only (as is true for isotropic and cubic symmetry).

3. Boundary condition $S_3=0$

The surface boundary condition $S_3=0$ [in which case there are no transmitted modes in medium (2)] can be satisfied basically by two different sets of conditions.

Type *s*:

$$A_i=B_i=C_i=\cdots=0,\quad i=1,2,3 \tag{2.39}$$

with consequently no constraint on $\dot{\Psi}_i,\dot{\Psi}_{i,3},\ldots$.

Type *h*:

$$A_i\neq 0,\ B_i\neq 0,\ldots,\quad i=1,2,3 \tag{2.40}$$

with $\dot{\Psi}_i=0,\dot{\Psi}_{i,3}=0,\ldots$.

In either case we obtain $3\gamma(1)$ conditions sufficient to determine the amplitudes of the reflected modes in medium (1).

The boundary conditions of type *s* generalize the concept of a "free surface": In this case all the phenomenological parameters entering $A_i,B_i,\ldots$ in medium (2) may be thought to go to zero as $\eta\to 0$ for finite field Ψ_i. Continuity then requires $A_i,B_i,\ldots$ in medium (1) to be zero at the interface ("soft environment").

The boundary conditions of type *h* generalize the concept of a "hard-environment": In this case the phenomenological parameters in medium (2) all go to infinity as $\eta\to\infty$. In order that $\mathcal{L}$ according to (2.7) remains finite, the corresponding field terms must scale as $\eta^{-1/2}$ and thus go to zero. Continuity then requires $\dot{\Psi}_i\dot{\Psi}_{i,3},\ldots$ to be zero at the interface. One can also think of mixed model environments like $A_3=0$, $\dot{\Psi}_i=0$, $i=1,2,\ldots$. Such boundary conditions are well known in conventional elasticity theory.[21] We will verify this concept by applying it to a number of known scenarios before we use its power for generalizations.

III. PHENOMENOLOGICAL ELECTROMAGNETIC FIELD

In a nonconducting isotropic continuum the Lagrangian for the transverse electromagnetic field $\mathcal{E}^T=-\dot{\mathbf{A}}$ in terms of the vector potential A_i (Coulomb gauge div $\mathbf{A}=0$, scalar potential $\Phi=0$, and SI units) can be taken as

$$\mathcal{L}(\dot{A}_i, A_{i,j})=\mathcal{L}_0(\dot{A}_i)+\frac{1}{2}\frac{\partial^2\mathcal{L}}{\partial A_{i,j}\partial A_{i',j'}}\bigg|_0 A_{i,j}A_{i',j'} \tag{3.1}$$

with

$$\mathcal{L}_0=\frac{\epsilon_0}{2}(1+\chi)\dot{A}_i\dot{A}_i \tag{3.2}$$

and

$$\frac{\partial^2\mathcal{L}}{\partial A_{i,j}\partial A_{i',j'}}\bigg|_0 \equiv -D_{ij|i'j'} , \tag{3.3}$$

with

$$D_{ij|ij}=\frac{1}{\mu_0}\frac{1}{1+\chi_m}\quad\text{with } D_{ij|ji}=-D_{ij|ij} . \tag{3.4}$$

The phenomenological parameters are thus controlled by the electric susceptibility χ and the magnetic susceptibility χ_m. The conjugate field is

$$\frac{\partial\mathcal{L}}{\partial\dot{A}_i}=\epsilon_0(1+\chi)\dot{A}_i=-D_i \tag{3.5}$$

and the equation of motion ("Helmholtz-equation"[22]) reads

$$\Delta A_i-\frac{(1+\chi)(1+\chi_m)}{c^2}\frac{\partial^2}{\partial t^2}A_i=0 , \tag{3.6}$$

where $\mu_0\epsilon_0=1/c^2$ has been used. This equation of motion is easily generalized for spatially dependent dielectrics $\chi(\mathbf{x})$. The parameters χ and χ_m can also be taken to define a heterojunction at $r_3=0$ (cf. dielectric or magnetic superstructures[12,23]). The pertinent continuity conditions are derived from the continuity of [cf. (2.36)]

$$S_3=-a_i^3\dot{A}_i \tag{3.7}$$

with

$$a_i^j = \frac{\partial \mathcal{L}}{\partial A_{i,j}} = \frac{1}{\mu_0}\frac{1}{1+\chi_m}(A_{i,j} - A_{j,i}) \;. \tag{3.8}$$

As the magnetic field is

$$\mathbf{H} = \frac{1}{\mu_0}\frac{1}{1+\chi_m}\,\mathrm{curl}\,\mathbf{A} \;, \tag{3.9}$$

the continuity of a_i^3, $i=1,2$, implies

$$H_i(2) = H_i(1), \quad i=1,2 \tag{3.10}$$

and the continuity of $\dot{A}_i$, $i=1,2$,

$$\mathcal{E}_i(2) = \mathcal{E}_i(1) \;, \tag{3.11}$$

i.e., the tangential components of $\mathcal{E}$ and $\mathbf{H}$ are continuous, as is well known. There is no constraint on $\mathcal{E}_3$, as $a_3^3 = 0$.

IV. PHENOMENOLOGICAL SCHRÖDINGER FIELDS

A. Scalar field

Neglecting spin we first consider the scalar complex Schrödinger field $\Psi(\mathbf{r},t)$ and $\Psi(\mathbf{r},t)^*$. Their Lagrangian, bilinear in Ψ and Ψ^*, can formally be defined by ($\gamma=1$)

$$\mathcal{L} = \mathcal{L}_0 + \left.\frac{\partial^2\mathcal{L}}{\partial\Psi^*\partial\Psi}\right|_0 \Psi^*\Psi + \left[\left.\frac{\partial^2\mathcal{L}}{\partial\Psi^*_{,j}\partial\Psi}\right|_0 \Psi^*_{,j}\Psi + \mathrm{c.c.}\right] + \left.\frac{\partial^2\mathcal{L}}{\partial\Psi^*_{,j}\partial\Psi_{,j'}}\right|_0 \Psi^*_{,j}\Psi_{,j'} \;, \tag{4.1}$$

where

$$\mathcal{L}_0 = -\frac{i\hbar}{2}\dot{\Psi}^*\Psi + \mathrm{c.c.} \tag{4.2}$$

For cubic symmetry all parameters are zero except

$$\left.\frac{\partial^2\mathcal{L}}{\partial\Psi^*\partial\Psi}\right|_0 = -V_0 \;, \qquad \left.\frac{\partial^2\mathcal{L}}{\partial\Psi^*_{,j}\partial\Psi_{,j'}}\right|_0 = -\frac{\hbar^2}{2m}\delta_{jj'} \;. \tag{4.3}$$

In this case the resulting Lagrange equations are just the usual time-dependent Schrödinger equation for Ψ and Ψ^*, respectively, interpreted as a classical wave equation.[24] On this fundamental level of description homogeneity means constant external potential V_0. An inhomogeneous structure model then amounts to defining a spatially dependent potential, while the mass m remains a fundamental constant: This does not change the pertinent equation of motion. Heterojunctions appear if the otherwise constant V_0 jumps on a plane interface, say $r_3=0$. The behavior of the Schrödinger field is then controlled by the continuity condition for

$$S_3 = -a^3\dot{\Psi} + \mathrm{c.c.} \tag{4.4}$$

with

$$a^j = \frac{\partial\mathcal{L}}{\partial\Psi^*_{,j}} = \frac{\hbar^2}{2m}\Psi_{,j} \;, \tag{4.5}$$

implying (for a nonsingular interface)

$$\Psi_{,3}(2) = \Psi_{,3}(1) \tag{4.6}$$

and the condition

$$\Psi(1) = \Psi(2)$$

(for any eigenmode $\dot{\Psi} \propto \Psi$). On a length $\Delta r \gg L_0$ (the interatomic distance) lattice electrons within a given band may be described by an effective Schrödinger field with

$$\left.\frac{\partial^2\mathcal{L}}{\partial\Psi^*\partial\Psi}\right|_0 = -E_g \;, \qquad \left.\frac{\partial^2\mathcal{L}}{\partial\Psi^*_{,j}\partial\Psi}\right|_0 = -A_j \;, \qquad \left.\frac{\partial^2\mathcal{L}}{\partial\Psi^*_{,j}\partial\Psi_{,j}}\right|_0 = -B_{jj'} \;. \tag{4.7}$$

Here $B_{ii'}$ denotes the reciprocal effective-mass tensor and E_g the band edge. For cubic symmetry $A_j=0$ and $B_{jj'} = (\hbar^2/2m^*)\delta_{jj'}$. Nonparabolicity can easily be accounted for by including higher-order derivatives ($\gamma>1$). With constant E_g and $B_{ii'}$ the phenomenological structure is now considered homogeneous: The lattice periodicity (and, correspondingly, the lattice-periodic part of the field modes) is no longer resolved. This is the well-known envelope function approximation.[9,10] Inhomogeneity on this longer length scale now means to let E_g and $B_{jj'}$ depend on space. This leads to the "generalized" Schödinger equation

$$i\hbar\dot{\Psi} + \frac{d}{dr_{j'}}(B_{jj'}\Psi_{,j}) - E_g(\mathbf{r})\Psi = 0 \;. \tag{4.8}$$

Heterojunctions are then controlled by the continuity condition $\Psi(1)=\Psi(2)$ and

$$a^3(2) = B_{3j}(2)\Psi_{,j}(2) = B_{3j}(1)\Psi_{,j}(1) = a^3(1) \;, \tag{4.9}$$

which, for an isotropic or cubic material, reduces to the relation[10]

$$\frac{1}{m^*}(2)\Psi_{,3}(2) = \frac{1}{m^*}(1)\Psi_{,3}(1) \;. \tag{4.10}$$

The justification of this equation has so far been rather unsatisfying.[25,26,20] Our approach can be applied to even longer length scales: For $\Delta r \gg L_1$ (the repetition length of a superlattice) the superlattice may be considered to define the homogeneous reference structure, so that for a heterojunction of superlattices one may wish to study the behavior of minibands.

B. Vector field

The phenomenological Schrödinger field can be extended also to multicomponent fields $\Psi_i(\mathbf{r},t)$, $i=1,2,\ldots,$ in order to account for a multiple band structure, such as, e.g., heavy-hole and light-hole bands in semiconductors. The corresponding parameter tensors are constrained by the appropriate point symmetry requirements. Such a procedure can be viewed as a real-space formulation of the Kohn-Luttinger approach in momentum space. Let us consider the field $\Psi_i(\mathbf{r},t)$, $i=1,2,3$, where Ψ_i transforms like r_i. Generalizing (4.1), the respective Lagrangian is (again up to first-ordr derivatives)

$$\mathcal{L}^{(2)}=\mathcal{L}_0+\left.\frac{\partial^2\mathcal{L}}{\partial\Psi_i^*\partial\Psi_{i'}}\right|_0\Psi_i^*\Psi_{i'} +\left[\left.\frac{\partial^2\mathcal{L}}{\partial\Psi_{i,j}^*\partial\Psi_{i'}}\right|_0\Psi_{i,j}^*\Psi_{i'}+\text{c.c.}\right] +\left.\frac{\partial^2\mathcal{L}}{\partial\Psi_{i,j}^*\partial\Psi_{i',j'}}\right|_0\Psi_{i,j}^*\Psi_{i',j'}\ , \quad (4.11)$$

where

$$\mathcal{L}_0=-\frac{i\hbar}{2}\dot{\Psi}_i^*\Psi_i+\text{c.c.}\ ,$$
$$\left.\frac{\partial^2\mathcal{L}}{\partial\Psi_i^*\partial\Psi_{i'}}\right|_0=-B_{ii'}\ ,$$
$$\left.\frac{\partial^2\mathcal{L}}{\partial\Psi_{i,j}^*\partial\Psi_{i'}}\right|_0=-C_{ij|i'}\ , \quad (4.12)$$
$$\left.\frac{\partial^2\mathcal{L}}{\partial\Psi_{i,j}^*\partial\Psi_{i',j'}}\right|_0=-D_{ij|i'j'}\ .$$

For cubic symmetry we have from (2.8) and Ref. 27

$$B_{ii'}=V_0\delta_{ii'},\quad C_{ij|i'}=C_{i|i'j'}=0,\quad D_{ii|ii}=\alpha,$$
$$D_{ij|ij}=D_{ij|ji}=\beta,\quad i\neq j \quad (4.13)$$
$$D_{ii|jj}=\gamma,\quad i\neq j\ .$$

Here V_0 is the potential energy and α,β,γ are the Kohn-Luttinger parameters (describing the light-hole and heavy-hole dispersion without spin). $D_{ij|i'j'}$ is in complete analogy with the fourth-rank elastic tensor (see next section). The equations of motion for the Ψ_i read

$$i\hbar\dot{\Psi}_i+\frac{\hbar^2}{2}\frac{d}{dr_j}(D_{ij|i'j'}\Psi_{i',j'})-V_0\Psi_i=0\ . \quad (4.14)$$

The continuity conditions are now

$$\Psi_i(2)=\Psi_i(1)\ ,$$
$$a_i^3(2)=a_i^3(1),\quad i=1,2,3 \quad (4.15)$$

where

$$a_i^j=\frac{\partial\mathcal{L}}{\partial\Psi_{i,j}}=-D_{ij|i'j'}\Psi_{i',j'}\ , \quad (4.16)$$

so that

$$-a_i^3=\beta(\Psi_{i,3}+\Psi_{3,i}),\quad i=1,2$$
$$-a_3^3=\alpha\Psi_{3,3}+\gamma(\Psi_{2,2}+\Psi_{1,1})\ .$$

Similar continuity conditions have been derived in Ref. 28. For lower symmetry the tensor C may also contribute giving rise to k linear terms in the dispersion and modifications in the continuity conditions.

V. MULTIPLE DISPLACEMENT FIELDS

An exposition of the Lagrangian formulation including multipole displacement fields can be found in Ref. 29. However, for the treatment of higher-order derivatives (dispersive corrections) in a layered material we have to focus on the concept of local (tensorial) parameter fields, which carry the local point symmetry as well as the material invariance constraints.

A. Invariance properties

Let us finally apply phenomenological field theory to multicomponent displacement fields $u_i^\nu(\mathbf{r},t)$, where ν relates, in the atomistic structure model, to different atomic units (mass M_ν) within the elementary lattice cell (volume v_c). On a length scale $\Delta r\gg a$ the discrete periodic character may be ignored. The Lagrange model in harmonic approximation reads [cf. (2.4) and (2.7)]

$$2\mathcal{L}^{uu}=\sum_{\nu\nu'}\int d^4\xi\,\beta_{ii'}^{\nu\nu'}(\mathbf{x}^s,\xi)u_i^\nu(\mathbf{x}^s+\tfrac{1}{2}\xi)u_{i'}^{\nu'}(\mathbf{x}^s-\tfrac{1}{2}\xi)\ , \quad (5.1)$$

with the expansion (in "standard form"; see Sec. II A)

$$2\mathcal{L}^{uu}=2\mathcal{L}_0-B_{ii'}^{\nu\nu'}u_i^\nu u_{i'}^{\nu'}-C_{i|i'j'}^{\nu\nu'}u_i^\nu u_{i',j'}^{\nu'} -D_{ij|i'j'}^{\nu\nu'}u_{i,j}^\nu u_{i',j'}^{\nu'}-\cdots \quad (5.2)$$

and

$$2\mathcal{L}_0^{uu}=\rho_\nu\dot{u}_i^\nu\dot{u}_i^\nu\ , \quad (5.3)$$
$$\rho_\nu=M_\nu/v_c\ , \quad (5.4)$$
$$\rho_0=\sum_\nu\rho_\nu\ . \quad (5.5)$$

As before, the parameters are constrained by point symmetry. "Spatial invariance,"[30] however, imposes additional relations: For a rigid translation $u_i^{(\nu)}\to u_i^{(\nu)}+\delta R_i$ we require

$$\mathcal{L}^{uu}[u_i^{(\nu)}+\delta R_i]-\mathcal{L}^{uu}[u_i^{(\nu)}]=\delta Q=0\ , \quad (5.6)$$

which means for arbitrary displacements u_i^ν,

$$\delta Q=\sum_{\nu\nu'}\int\beta_{ii'}^{\nu\nu'}(\mathbf{r}^s,\xi)[u_i^\nu(\mathbf{r}^s-\tfrac{1}{2}\xi)\delta R_i' +u_{i'}^{\nu'}(\mathbf{r}^s+\tfrac{1}{2}\xi)\delta R_i]d^3\xi=0\ . \quad (5.7)$$

We expand this condition up to second-order terms in the derivatives of the displacement field. For higher-order terms the standard form of $\mathcal{L}$ (see Sec. II A) automatically fulfills homogeneity. $\delta Q=0$ should hold for arbitrary δR_i and therefore

$$\sum_\nu\int d^3\xi\,\beta_{ii'}^{\nu\nu'}u_{i'}^{\nu'}(\mathbf{r}^s)=\sum_\nu B_{ii'}^{\nu\nu'}u_{i'}^{\nu'}(\mathbf{r}^s)=0\ ,$$
$$\tfrac{1}{2}\sum_\nu\int d^3\xi\,\beta_{ii'}^{\nu\nu'}\xi_k u_{i',k'}^{\nu'}(r^s)=\sum_\nu C_{i|i'k'}^{\nu\nu'}u_{i',k'}^{\nu'}(\mathbf{r}^s)=0 \quad (5.8)$$

results for any displacement field. These subsidiary conditions can be taken care of by the coupling constants if we let

$$\sum_\nu B_{ii'}^{\nu\nu'}=0,\quad \sum_\nu C_{i|i'k'}^{\nu\nu'}=0\ . \quad (5.9)$$

For the invariance under rigid body rotation of angle α, we insert

$$\delta R_i(\alpha)=d\alpha\,\omega_{im}r_m \tag{5.10}$$

into (5.7) with the antisymmetric tensor $\omega_{im}=-\omega_{mi}$ and $r_m=r_m^s+\xi_m$. The expansion up to first-order field derivatives leads again for arbitrary u_i^ν to

$$\sum_\nu \int d^4\xi\,\beta_{ii'}^{\nu\nu'}\xi_m\xi_{k'}u_{i',k'}^{\nu'}\omega_{im}=0\ , \tag{5.11}$$

which should hold for any ω_{im}, so that

$$\sum_\nu \int d^4\xi\,\beta_{ii'}^{\nu\nu'}\xi_m\xi_{k'}u_{i',k'}^{\nu'}\omega_{im}=u_{i',k'}^{\nu'}\sum_\nu D_{im|i'k'}^{\nu\nu'}\omega_{im}=0\ . \tag{5.12}$$

This constraint is, again, taken care of by the coupling tensors, if

$$D_{im|i'k'}^{\nu\nu'}=D_{mi|i'k'}^{\nu\nu'}\ . \tag{5.13}$$

Corresponding relations for higher-order terms are obtained, e.g.,

$$F_{ikl|i'k'l'}^{\nu\nu'}=F_{kil|i'k'l'}^{\nu\nu'}\ , \tag{5.14}$$

etc.

B. Center-of-mass and relative displacement fields

Without loss of generality we restrict ourselves to a twofold displacement field (corresponding to a lattice unit cell with two atoms, typical for semiconductors). In analogy to the Jacobi coordinates (see Sec. II A) we may then introduce the center-of-mass (COM) displacement field[31,29]

$$s_i=\sum_\nu \frac{\rho_\nu}{\rho_0}u_i^\nu \tag{5.15}$$

and the relative displacement field

$$w_i=u_i^1-u_i^2\ . \tag{5.16}$$

Though, in general, these two fields do not decouple (see below), they serve as long-wavelength approximations of the acoustic and optical displacement fields, respectively, and appear in virtually all electron-phonon coupling models.

Transforming the Lagrangian (5.1), to these new fields, we obtain

$$\mathcal{L}^{uu}=\mathcal{L}_{\rm kin}^s+\mathcal{L}_{\rm kin}^w-V^{ss}-V^{sw}-V^{ww}\ , \tag{5.17}$$

where

$$\mathcal{L}_{\rm kin}^s=\tfrac{1}{2}\rho_0\dot{s}_i\dot{s}_i,\quad \mathcal{L}_{\rm kin}^w=\tfrac{1}{2}\rho_{\rm eff}\dot{w}_i\dot{w}_i \tag{5.18}$$

are the kinetic energy terms with

$$\rho_{\rm eff}=\left[\frac{1}{\rho_1}+\frac{1}{\rho_2}\right]^{-1} \tag{5.19}$$

and

$$\pi_i^s=\rho_0\dot{s}_i,\quad \pi_i^w=\rho_{\rm eff}\dot{w}_i\ . \tag{5.20}$$

The leading terms of the potential-energy density for the s field are

$$2V^{ss}=D_{ij|i'j'}^{ss}s_{i,j}s_{i',j'}+2E_{ij|i'j'k'}^{ss}s_{i,j}s_{i',j'k'}+F_{ijk|i'j'k'}^{ss}s_{i,jk}s_{i',j'k'}\ , \tag{5.21}$$

where

$$D_{ij|i'j'}^{ss}=-\left.\frac{\partial\mathcal{L}}{\partial s_{i,j}\partial s_{i',j'}}\right|_0 \tag{5.22}$$

denotes the elastic tensor, while

$$E_{ij|i'j'k'}^{ss}=-\left.\frac{\partial\mathcal{L}}{\partial s_{i,j}\partial s_{i',j'k'}}\right|_0 \tag{5.23}$$

and

$$F_{ijk|i'j'k'}^{ss}=-\left.\frac{\partial\mathcal{L}}{\partial s_{i,jk}\partial s_{i',j'k'}}\right|_0 \tag{5.24}$$

account for dispersive corrections. The leading terms for the w field are

$$2V^{ww}=B_{i|i'}^{ww}w_iw_{i'}+2C_{ij|i'}^{ww}w_{i,j}w_{i'}+D_{ij|i'j'}^{ww}w_{i,j}w_{i',j'} \tag{5.25}$$

with

$$B_{i|i'}^{ww}=-\left.\frac{\partial\mathcal{L}}{\partial w_i\partial w_{i'}}\right|_0\ , \tag{5.26}$$

etc. Finally, the coupling between the s and w field is described by

$$V^{sw}=C_{ij|i'}^{sw}s_{i,j}w_{i'}+D_{ij|i'j'}^{sw}s_{i,j}w_{i',j'}+\tilde{D}_{ijk|i'}^{sw}s_{i,jk}w_{i'}+E_{ijk|i'j'}^{sw}s_{i,jk}w_{i',j'}\ . \tag{5.27}$$

We see that s_i is a cyclic field variable while w_i is not. The transformed parameters D^{ss}, F^{ss}, etc., can be expressed in terms of the original parameters as given in the Appendix. The invariance properties of the latter [cf. (5.13)] thus imply

$$D_{ij|i'j'}^{ss}=D_{ji|i'j'}^{ss}=D_{ij|j'i'}^{ss}\ . \tag{5.28}$$

Corresponding relations hold for D^{sw} and D^{ww}. Furthermore,

$$C_{ij|i'}^{ww}=C_{ji|i'}^{ww}\ ,\quad E_{ijk|i'j'}^{ss}=E_{jik|j'i'}^{ss}\ . \tag{5.29}$$

Antisymmetry obtains

$$C_{ij|i'}^{ww}=-C_{i'j|i}^{ww}\ ,\quad E_{ijk|i'j'}^{ss}=-E_{i'j'k|ij}^{ss} \tag{5.30}$$

using (2.8).

C. Lagrange equations

The Lagrange equation of motion reads (within a homogeneous layer)

$$\rho_0\ddot{s}_i-D_{ij|i'j'}^{ss}s_{i',j'j}-2E_{i'jk|ij'}^{ss}s_{i',jkj'}+F_{ijk|i'j'k'}^{ss}s_{i',j'k'jk}=S_i^{sw}\ . \tag{5.31}$$

E and F describe dispersive corrections. The source term on the right-hand side is

$$S_i^{sw}=C_{ij|i'}^{sw}w_{i',j}+D_{ij|i'j'}^{sw}w_{i',j'j}-\tilde{D}_{ijk|i'}^{sw}w_{i',jk}-E_{ijk|i'j'}^{sw}w_{i',jj'k} . \tag{5.32}$$

Similarly we obtain for the w field

$$\rho_{\text{eff}}\ddot{w}_i+B_{ii'}^{ww}w_{i'}+2C_{i'j'|i}^{ww}w_{i',j'}-D_{im|i'j'}^{ww}w_{i',j'm}=S_i^{ws} , \tag{5.33}$$

with

$$S_i^{ws}=-C_{i'j'|i}^{sw}s_{i',j'}+D_{ij|i'j'}^{sw}s_{i',j'j}-\tilde{D}_{i'j'k'|i}^{sw}s_{i',j'k'} . \tag{5.34}$$

The existence of similar equations of motion for the w field has been previously postulated.[32] If allowed by point symmetry, the C^w terms could be responsible for k linear terms in $w^2(\mathbf{k})$ (as has been discussed for the vector Schrödinger field). S_i^{sw} and S_i^{ws} describe optical- and acoustic-mode mixing, as discussed in the next section.

VI. INTERACTIONS BETWEEN DIFFERENT FIELDS

Our procedure of obtaining continuity conditions also applies to interacting fields $\Psi_i^{(\nu)}$, $\nu=1,2,\ldots$, as long as we restrict ourselves to bilinear terms. Examples for such coupled modes are the mixed center-of-mass and relative displacement modes ("phonons" proper) and the mixed photon field and polarization field modes ("polaritons"). For the latter an additional boundary condition (ABC) problem has long since been recognized if the (mechanical) polarization mode shows dispersion ($\gamma\geq 1$):[33–35] This problem is easily resolved by our prescription provided the polarization field can be considered local (i.e., expandable in terms of finite-order derivatives).

A. Mixed COM and relative displacement modes

Since the $\mathbf{s}$ and $\mathbf{w}$ fields interact [see (5.27)], the proper phonon eigenmodes Ψ of the bulk system have to be formulated in the six-dimensional (direct sum) space with unit polarization vectors e_n, $n=1,2,\ldots 6$, which are defined, as before, over three-dimensional real space. The coupling will change the respective dispersion relations (as would do also higher derivatives in the separate fields) but, in particular, will change the original set of eigenvectors for the $\mathbf{u}_1,\mathbf{u}_2$ displacement fields:

$$\mathbf{e}_1=\mathbf{e}^s+\frac{\rho_2}{\rho_0}\mathbf{e}^w,\quad \mathbf{e}_2=\mathbf{e}^s-\frac{\rho_1}{\rho_0}\mathbf{e}^w , \tag{6.1}$$

where [$\mathbf{e}^s=(e_1,e_2,e_3)$, $\mathbf{e}^w=(e_4,e_5,e_6)$]. Recent experiments[36] allow us to determine these eigenvectors, from which the $\mathbf{s}$-$\mathbf{w}$ coupling could, in turn, be estimated. We now consider the continuity conditions for these mixed modes. The plane-wave ansatz as given in (2.32) is for $\gamma(1)=\gamma(2)$ generalized to

$$\Psi_n(1)=e^{i(\mathbf{k}_\parallel\mathbf{R}-\omega t)}\times\left\{e_n^0 e^{ik_3^0 r_3}+\sum_{l=1}^{6}\sum_{m=1}^{\gamma}\varphi^{lm}(1)e_n^{lm}e^{-ik_3^m r_3}\right\} , \quad r_3\leq 0 \tag{6.2}$$

$$\Psi_n(2)=e^{i(\mathbf{k}_\parallel\mathbf{R}-\omega t)}\sum_{l=1}^{6}\sum_{m=1}^{\gamma}\varphi^{lm}(2)e_n^{lm}e^{ik_3^m r_3} , \quad r_3\geq 0, n=1\ldots 6 ,$$

where e_n^{lm} denotes the six-dimensional (normalized) eigenvectors corresponding to frequency ω and $\mathbf{k}_\parallel$ in regions (1) and (2), respectively. The 12γ amplitudes $\varphi^{lm}(1),\varphi^{lm}(2)$ have to be determined. Observing that $\mathbf{s}=(\Psi_1,\Psi_2,\Psi_3)$ and $\mathbf{w}=(\Psi_4,\Psi_5,\Psi_6)$, this ansatz must satisfy the $6\times 2\gamma$ continuity conditions, (2.38), i.e., $\Psi_n(1)=\Psi_n(2),\Psi_{n,3}(1)=\Psi_{n,3}(2),\ldots$, with $n=1,2,\ldots 6$ and

$$A_n(1)=A_n(2),\quad B_n(1)=B_n(2) , \tag{6.3}$$

where $A_n,B_n,\ldots$ are decomposed according to (2.37) with

$$a_i^3=-D_{i3|i'j'}^{ss}\Psi_{i',j'}-2E_{i3|i'j'k'}^{ss}\Psi_{i',j'k'} -C_{i3|i'}^{sw}\Psi_{i'+3}-D_{i3|i'j'}^{sw}\Psi_{i'+3,j'}-\frac{d}{dr_j}b_i^{3j}\cdots ,$$

$$b_i^{3j}=-2E_{i'j'|i3j}^{ss}\Psi_{i',j'}-F_{i3j|i'j'k'}^{ss}\Psi_{i',j'k'}-\frac{d}{dr_l}c_i^{3jl}$$

$$\vdots \tag{6.4}$$

$$a_{i+3}^3=-2C_{i3|i'}^{ww}\Psi_{i'+3}-D_{i3|i'j'}^{ww}\Psi_{i'+3,j'} -D_{i'j'|i3}^{sw}\Psi_{i',j'}-\frac{d}{dr_j}b_m^{3j}\cdots$$

$$\vdots \tag{6.5}$$

As we see from (6.4) and (6.5) there is an optical- and acoustic-mode mixing also due to the continuity conditions.

B. Longitudinal polar phonon modes

For a polar displacement field we have to include the interaction with the electric field $\mathscr{E}_i$, given by the Lagrangian density[11]

$$\mathcal{L}^{\epsilon u}=\mathcal{L}^{\epsilon u}(u_i^\nu,u_{i,j}^\nu,\ldots,\mathscr{E}_{i'})=\mathscr{E}_i\tilde{p}_i , \tag{6.6}$$

where $\tilde{p}_i$ denotes the polarization field with the expansion

$$\tilde{p}_i=\epsilon_0(\epsilon_\infty-1)\mathscr{E}_i+B_{ii'}^{\epsilon\nu}u_{i'}^\nu+C_{i|i'j'}^{\epsilon\nu}u_{i',j'}^\nu+\cdots . \tag{6.7}$$

ϵ_∞ takes into account the electronic background. Transformation to the $\mathbf{s}$ and $\mathbf{w}$ fields implies

$$\tilde{p}_i=\tilde{p}_i^s+\tilde{p}_i^w+\epsilon_0(\epsilon_\infty-1)\mathscr{E}_i , \tag{6.8}$$

with

$$\tilde{p}_i^s=C_{i|i',j'}^{\epsilon s}+D_{i|i'j'k'}^{\epsilon s}s_{i',j'k'}+\cdots ,$$
$$\tilde{p}_i^w=B_{i|i'}^{\epsilon w}w_{i'}+C_{i|i'j'}^{\epsilon w}w_{i',j'}+\cdots . \tag{6.9}$$

Here

$$C_{i|i'j'}^{\epsilon s}=\left.\frac{\partial^2\mathcal{L}^{\epsilon s}}{\partial s_{i',j'}\partial\mathscr{E}_i}\right|_0=C_{i|j'i'}^{\epsilon s} \tag{6.10}$$

is the first-order piezoelectric tensor.[11] The interaction $\mathcal{L}^{u\epsilon}$ influences the equations of motion of the mechanical fields $\mathbf{s}$ and $\mathbf{w}$ and of the electric field $\mathscr{E}$: The right-hand side of (5.31) is supplemented by

$$S_{i'}^{\epsilon s}=-(C_{i|i'j'}^{\epsilon s}\mathcal{E}_i)_{,j'}+(D_{i|i'j'k'}^{\epsilon s}\mathcal{E}_i)_{,j'k'} \quad (6.11)$$

and the right-hand side of (5.33) by

$$S_{i'}^{\epsilon w}=B_{ii'}^{\epsilon w}\mathcal{E}_i-(C_{i|i'j'}^{\epsilon w}\mathcal{E}_i)_{i,'}+\cdots . \quad (6.12)$$

The electric field may be split into a longitudinal ($\mathrm{curl}\mathcal{E}^L=0$) and a transverse part ($\mathrm{div}\mathcal{E}^T=0$). In Coulomb gauge $\mathrm{div}\,\mathbf{A}=0$, the longitudinal part is given by

$$\mathcal{E}_i^L=-\Phi_{,i} \quad (6.13)$$

and controlled by the equation of motion of the scalar potential Φ,

$$\Delta\Phi=\frac{1}{\epsilon_0}\mathrm{div}\tilde{\mathbf{p}} , \quad (6.14)$$

so that

$$\mathrm{div}\mathcal{E}^L=-\frac{1}{\epsilon_0}\mathrm{div}\tilde{\mathbf{p}} \quad (6.15)$$

or

$$\mathrm{div}(\epsilon_0\mathcal{E}^L+\tilde{\mathbf{p}})=\mathrm{div}\mathbf{D}=0 , \quad (6.16)$$

which can be satisfied by

$$\epsilon_0\epsilon_\infty\mathcal{E}^L=-(\tilde{\mathbf{p}}_L^s+\tilde{\mathbf{p}}_L^w) . \quad (6.17)$$

In this way $\mathcal{E}^L$ can be eliminated from the respective equations of motion. Neglecting **s**-**w** coupling, the $\gamma=1$ version of the effective equations of motion for $\mathbf{w}^L$ reads

$$\rho_0\ddot{w}_i^L+B_{ii'}^{ww}w_{i'}^L+2C_{i'j'|i}^{ww}w_{i',j'}^L-D_{ij|i'j'}^{ww}w_{i',j'j}^L$$
$$=-\frac{2\epsilon_\infty-1}{\epsilon_0\epsilon_\infty^2}[B_{ii'}^{\epsilon w}(B_{i'j}^{\epsilon w}w_j^L+C_{i'jk}^{\epsilon w}w_{j,k}^L)$$
$$-C_{ii'j'}^{\epsilon w}(B_{i'j}^{\epsilon w}w_{j,j'}^L+C_{i'jk}^{\epsilon w}w_{j,kj'}^L)] . \quad (6.18)$$

For all third-order tensors $C=0$ we obtain the usual shifted LO mode. In any case, the number of continuity conditions required is the same as without polar coupling. For the $\mathbf{w}^L$ fields with a plane wave being incident perpendicular to the surface, these conditions are, from (2.37) and (2.38) (cf. Refs. 37 and 38),

$$w_3^L(1)=w_3^L(2),\quad a_3^3(1)=a_3^3(2) , \quad (6.19)$$

where

$$a_3^3=-2C_{33|3}^{ww}w_3^L-D_{33|33}^{ww}w_{3,3}^L$$
$$-\frac{2\epsilon_\infty-1}{\epsilon_0\epsilon_\infty^2}C_{333}^{\epsilon w}(B_{33}^{\epsilon w}w_3^L+C_{333}^{\epsilon w}w_{3,3}^L) , \quad (6.20)$$

which is for all tensors $C=0$ just the mechanical boundary condition.

C. Transverse modes: Phonon polariton

Since the value of the electromagnetic wave vector is very small, the coupling of the **s** and **w** fields may be neglected in this region. Though, in general, there is a coupling of the transverse electromagnetic field to both displacements **s** and **w**, we restrict ourselves to the **w** field. The Lagrangian for these modes reads

$$\mathcal{L}=\mathcal{L}^{\epsilon\epsilon}+\mathcal{L}^{ww}+\mathcal{E}_i\tilde{p}_i , \quad (6.21)$$

with $\mathcal{L}^{\epsilon\epsilon}$ given by (3.1) with $\chi_m=1$, $\chi=\epsilon_\infty-1=\mathrm{const}$, and

$$\tilde{p}_i=\epsilon_0(\epsilon_\infty-1)\mathcal{E}_i+B_{i|i'}^{\epsilon w}w_{i'}+C_{i|i'j'}^{\epsilon w}w_{i',j'}+\cdots . \quad (6.22)$$

The equations of motion for the transverse parts with $\gamma=1$ (for either field) read

$$\Delta A_i^T-\frac{1}{c^2}\ddot{A}_i^T=-\mu_0\dot{\tilde{p}}_i^T$$
$$\rho\ddot{w}_i^T-B_{ii'}^{ww}w_{i'}^T-C_{i'ji}^{ww}w_{i',j}^T+D_{iji'j'}^{ww}w_{i',j'j}^T$$
$$=-\dot{A}_i\frac{\partial\tilde{p}_{i'}^T}{\partial w_i^T}-\frac{d}{dr_j}\left[\frac{\partial\tilde{p}_{i'}^T}{\partial w_{i,j}^T}\dot{A}_i^T\right] . \quad (6.23)$$

The respective space for the mode solutions of (6.23) is now the six-dimensional polariton vector space $\Psi=(\mathbf{A},\mathbf{w})$. Keeping only terms in **w** ($\gamma=0$), we recover the result as discussed in Ref. 31. To get the appropriate conditions we make an ansatz for the polariton modes Ψ in the same way as we did in Sec. VI A.

The scenario of a plane wave $\mathcal{E}^T=-\dot{\mathbf{A}}^T$ being incident perpendicular to a free surface (note that there would otherwise be mixing between longitudinal and transverse) leads us to the following constraints for the electromagnetic field $(A_1,A_2,A_3)=(\Psi_1,\Psi_2,\Psi_3)$:

$$\Psi_j(1)=\Psi_j(2),\quad a_j^3(1)=a_j^3(2) , \quad (6.24)$$

as before [cf. (3.8)]. Assuming a soft environment for the **w** field in medium (1), $(w_1,w_2,w_3)=(\Psi_4,\Psi_5,\Psi_6)$, the pertinent continuity conditions are [cf. (2.39)] with

$$a_{i+3}^3(1)=0,\quad i=1,2,3 \quad (6.25)$$

$$a_{i+3}^3=\frac{\partial\mathcal{L}}{\partial\Psi_{i+3,3}}=-C_{i3|i'}^{ww}\Psi_{i'+3}-D_{i3i'j}^{ww}\Psi_{i'+3,j}-C_{i3j}^{\epsilon w}\dot{\Psi}_j ,$$
$$i=1,2,3 . \quad (6.26)$$

We first discuss these terms for an isotropic or cubic material: In these cases C^{ww} and $C^{\epsilon w}$ are zero, and with the appropriate form of D^{ww} (6.26) reduces to $w_{i,3}^T=0$, $i=1,2$. This result coincides with the ABC's as discussed by Ting, Frankel, and Birman[39] for the exiciton polariton.

The ABC $w_i^T=0$ suggested by Pekar,[40] on the other hand, is recovered for a hard environment or "clamped surface" scenario [compare (2.40)]. In terms of the Schrödinger (or excitonic) field, this model assumes an infinite barrier at the surface. It is interesting to remark that if we drop the constraint of $\mathbf{C}^{ww}=0$, we would get generalized continuity conditions as linear combinations of the ones described above.[34] With $\mathbf{C}^{\epsilon w}\neq0$ the mechanical boundary condition explicitly depends on the lightwave amplitude. Instead of using these field expansions, the required continuity conditions can alternatively be obtained from a properly handled integral equation (see, e.g., Ref. 41).

VII. SUMMARY AND CONCLUSIONS

We have investigated the properties of dynamical fields in heterostructures, starting from a variational formulation. Including gradient terms higher than first order, we are able to take into consideration that most dynamical fields in solids are dispersive, as a consequence of the material properties. We have then introduced the concept of parameter fields describing the local couplings of the dynamical fields and their derivatives. While the bulk-material determines the point symmetry of the parameter fields, their tensor character is given by the order of the derivatives introduced: The higher the order, the "less local" the description becomes. Structural length scales specify the spatial dependence of the parameter fields. If these length scales are large enough in the case of heterostructures, the parameter fields are allowed to change discontinuously at the interfaces.

Our main object has been to derive the continuity conditions at a plane interface. Our systematic derivation is based on the conservation of the energy flux perpendicular to the interface and on the linearity of the equations of motion. Two different classes of surface models have been considered: The first class with zero energy flux comprises the hard and soft environment, which is illustrated for the displacement field by the free or clamped surface, respectively. For the second class with finite energy flux we have provided various examples for different field types: In the case of the electromagnetic field dielectric or magnetic heterostructures have been discussed. For the Schrödinger field we have shown that the spatial dependence of the effective mass is just another version of a parameter field, and also how it properly enters the continuity conditions. These considerations, have been generalized to a degenerate band structure (heavy-hole, light-hole bands), a situation which is formally equivalent to the longitudinal and transverse phonon branches. Further examples have been given for multiple phase displacement fields: We have derived boundary conditions for the optical phonon field (with dispersion). Finally, the procedure has been applied to interacting dynamical fields. In this case the respective eigenvector space is the direct sum of the subspaces of the noninteracting fields, while the continuity conditions are calculated as before, thus including the so-called additional boundary conditions. There is no ambiguity or additional degree of freedom in the choice of the proper continuity conditions. This is highlighted, e.g., by the additional boundary conditions for the electromagnetic field interacting with the polarization field. Once the model is defined, the conditions are conclusive in our description.

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APPENDIX: EFFECTIVE PARAMETERS

The parameters for the $\mathbf{s}$ and $\mathbf{w}$ fields can uniquely be expressed in terms of the original parameters for the $\mathbf{u}^\nu$ fields. They come in three groups.

(1) Parameters of any order not involving the $\mathbf{w}$ field are constructed according to

$$X^{ss\cdots s}=\sum_{\nu\nu'\nu''\cdots} X^{\nu\nu'\nu''\cdots}$$

for each matrix element. This means, e.g.,

$$C^{s\epsilon}_{ij|i'}=\sum_\nu \left.\frac{\partial^2\mathcal{L}}{\partial u^\nu_{i,j}\partial\epsilon_{i'}}\right|_0 ,$$

$$D^{s\epsilon}_{ijk|i'}=\sum_\nu \left.\frac{\partial^2\mathcal{L}}{\partial u^\nu_{i,jk}\partial\epsilon_{i'}}\right|_0 ,$$

$$D^{ss}_{ij|i'j'}=\sum_\nu \left.\frac{\partial^2\mathcal{L}}{\partial u^\nu_{i,j}\partial u^\nu_{i',j'}}\right|_0 .$$

D^{ss} is the elastic tensor. All symmetry requirements with respect to the Cartesian indices in the $\mathbf{u}^1/\mathbf{u}^2$ representation carry over to the $\mathbf{s}/\mathbf{w}$ representation.

(2) Parameters to any order linear in the $\mathbf{w}$ field are constructed according to

$$X^{ss\cdots w}=\frac{\rho_2}{\rho_0}\sum_{\nu\nu'\cdots} X^{\nu\nu'\cdots 1}-\frac{\rho_1}{\rho_0}\sum_{\nu\nu'\cdots} X^{\nu\nu'\cdots 2} .$$

Explicit examples are

$$B^{w\epsilon}_{ii'}=\left.\frac{\rho_2}{\rho_0}\frac{\partial^2\mathcal{L}}{\partial u^1_i\partial\epsilon_{i'}}-\frac{\rho_1}{\rho_0}\frac{\partial^2\mathcal{L}}{\partial u^2_i\partial\epsilon_{i'}}\right|_0 ,$$

$$D^{sw}_{ij|i'j'}=\frac{\rho_2}{\rho_0}\sum_\nu \left.\frac{\partial^2\mathcal{L}}{\partial u^\nu_{i,j}\partial u^1_{i',j'}}\right|_0-\frac{\rho_1}{\rho_0}\sum_\nu \left.\frac{\partial^2\mathcal{L}}{\partial u^\nu_{i,j}\partial u_{i',j'}{}^2}\right|_0 .$$

Only symmetry requirements with respect to the Cartesian indices of one and the same field carry over from the $\mathbf{u}^1/\mathbf{u}^2$ representation to the $\mathbf{s}/\mathbf{w}$ representation.

(3) Parameters to any order quadratic in the $\mathbf{w}$ field are constructed according to

$$X^{ss\cdots ww}=\left[\frac{\rho_2}{\rho_0}\right]^2\sum_{\nu\nu'\cdots} X^{\nu\nu'\cdots 11}+\left[\frac{\rho_1}{\rho_0}\right]^2\sum_{\nu\nu'\cdots} X^{\nu\nu'\cdots 22} -\frac{\rho_1\rho_2}{\rho_0^2}\sum_{\nu\nu'\cdots}(X^{\nu\nu'\cdots 12}+X^{\nu\nu'\cdots 21}) .$$

Explicit examples are

$$B^{ww}_{ii'}=\left[\frac{\rho_2}{\rho_0}\right]^2\left.\frac{\partial^2\mathcal{L}}{\partial u^1_i\partial u^1_{i'}}\right|_0+\left[\frac{\rho_1}{\rho_0}\right]^2\left.\frac{\partial^2\mathcal{L}}{\partial u^2_i\partial u^2_{i'}}\right|_0 -\frac{\rho_1\rho_2}{\rho_0^2}\left[\left.\frac{\partial^2\mathcal{L}}{\partial u^1_i\partial u^2_{i'}}\right|_0+\left.\frac{\partial^2\mathcal{L}}{\partial u^2_i\partial u^1_{i'}}\right|_0\right] ,$$

$$D^{w}_{iji'j'}=\left[\frac{\rho_2}{\rho_0}\right]^2\left.\frac{\partial^2\mathcal{L}}{\partial u^1_{i,j}\partial u^1_{i',j'}}\right|_0+\left[\frac{\rho_1}{\rho_0}\right]^2\left.\frac{\partial^2\mathcal{L}}{\partial u^2_{i,j}\partial u^2_{i',j'}}\right|_0 -\frac{\rho_1\rho_2}{\rho_0^2}\left[\left.\frac{\partial^2\mathcal{L}}{\partial u^1_{i,j}\partial u^2_{i',j'}}\right|_0+\left.\frac{\partial^2\mathcal{L}}{\partial u^2_{i,j}\partial u^1_{i',j}}\right|_0\right] .$$

In this pure $\mathbf{w}$ case, again, all symmetry requirements with respect to the Cartesian indices $i,j\ldots$ in the $\mathbf{u}^1/\mathbf{u}^2$ representation are the same as in the $\mathbf{s}/\mathbf{w}$ representation.

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