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Wave-quasi-particle dualism for surface acoustic waves: theory and applications

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Abstract Following along the line of the theory proposed initially at CFA-2010, this contribution presents the recent progress achieved in this trend of research. Here the focus is put on various cases of SH waves with perturbing effects due to the elastic non-linearity of the substrate, its viscosity, and the presence of a thin active film glued on top of the substrate. The problem of transmission-reflection at an interface between two elastic media is also considered as an example exhibiting the alternate wavelike and particle-like pictures of the solution. This interface may be a discontinuity with possible delamination, a slab of finite thickness, or a multi-layered structure.

1 Introduction

In recent works (e.g., [1], [2]), influenced by the theories of phonons in solid state physics and of solitons in mathematical physics, we have expanded a theory of *quasi-particles* that are associated with surface acoustic wave (SAW) modes. These particles we nicknamed “grains of SAWs”. This association akin to a dualism is obtained, once we know the continuum solution of the SAW problem, by exploiting the so-called canonical equations of conservation of wave momentum and energy - see [3] for this general concept. These equations are obtained by any means (e.g., application of Noether’s invariance theorem [4] in the case of nondissipative systems for which we know the Lagrangian; or direct manipulation of the standard balance laws in the presence of dissipation). The applied methodology consists in evaluating the expression of the “mass” and the accompanying “kinetic energy” of the associated quasi-particle. This is done by integrating the local conservation laws of wave momentum (cf. Brenig [5] for this notion) over a material volume that is representative of the studied wave motion. In propagation space this amounts to an average over one wavelength. Then one has to substitute for the known analytical wave solution in the resulting equations

2 Reminder: notions of conservation law, wave momentum and quasi-particle

There exists a fundamental difference between *field equations* that govern individual degrees of freedom of a physical system and *conservation laws* that pertain to the whole considered system. This difference was first made clear by Emmy Noether in her celebrated theorem of 1918 [4]. For instance, in the standard Cartesian tensorial index notation of continuum solid mechanics in small strains the *field equations* (so-called balance of - physical- linear momentum) read in the absence of body force and for a volume element

$$\frac{\partial}{\partial t}(\rho_0 \dot{u}_i) - \frac{\partial}{\partial x_j} \sigma_{ji} = 0, \quad (1)$$

where ρ_0 is the matter density at the reference configuration, u_i denotes the three components of

the displacement, \dot{u}_i denotes the corresponding velocity, and σ_{ji} stands for the symmetric Cauchy stress. Eq. (1) pertains to *the* displacement component u_i . In contrast, the local balance of energy governs *all* degrees of freedom simultaneously and reads in the absence of external source of energy and of heat conduction

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho_0 \dot{\mathbf{u}}^2 + W \right) - \frac{\partial}{\partial x_j} (\sigma_{ji} \dot{u}_i) = 0, \quad (2)$$

where W is the potential energy per unit volume. Eq. (2) in fact is a *true conservation law* for the considered thermo-mechanical physical system. It reflects its invariance under time translations. It is not the only conservation law as we should in parallel consider the invariance under spatial parametrization (material coordinates). The resulting equation is called the conservation of *material* (or pseudo-) *momentum* and generally reads [3]

$$\frac{\partial}{\partial t} P_i - \frac{\partial}{\partial x_j} b_{ji} = f_i^S, \quad (3)$$

where

$$P_i = -\rho_0 \dot{u}_j u_{j,i}, \quad b_{ji} = -\left(\frac{1}{2} \rho_0 \dot{\mathbf{u}}^2 - W \right) \delta_{ji} - \sigma_{jk} u_{k,i}. \quad (4)$$

Here b_{ji} is referred to as the Eshelby (material) stress, W is the free energy density, and the “force” source term f_i^S accounts for effects of true material inhomogeneities, thermal and anelastic effects, if any, all in the form of “*forces of inhomogeneity*” [3]. For a perfectly homogeneous (but possibly anisotropic) purely elastic body f_i^S vanishes identically and (3) becomes a *strict* (covariant) *conservation law* reflecting an invariance under translation of material coordinates. This case follows from the application of Noether’ theorem relating to the invariance under material space parametrization. Otherwise, Eq. (3) is deduced from the standard equations (1) through manipulations.

If Eq. (1) are traditionally used to solve static and dynamic (wave) problems on account of prescribed boundary and initial conditions, the additional equation (3) must be exploited in a

second step, such as in a post-processing procedure. In the present setting we propose to exploit Eq. (3) with a view to associating a quasi-particle vision to linear wave processes of a certain type (e.g., acoustic surface waves propagating on the top of a substrate once the analytical wavelike solutions is known). In particular, an interesting quantity here is the so-called quasi-particle (wave) momentum obtained by evaluating the average of P_i over a volume element most representative of the studied wave process, i.e., symbolically

$$P_i^{QP} = \langle P_i \rangle . \quad (5)$$

Then Eq. (3) will yield the “equation of motion” of the associated quasi-particle by integration over this volume. The same procedure is applied to the energy equation. The effective “mass” of the quasi-particle is evaluated in the procedure

3 SH and Bleustein-Gulyaev (BG) waves

3.1 Reminder

The case of Rayleigh SAWs was studied in Ref. [2] together with various types of perturbations. Shear-horizontal (SH) SAWs are in principle much simpler than Rayleigh SAWs because they involve only *one* displacement component u_3 orthogonal to the sagittal plane Π_S of coordinates (x_1, x_2) , but they exist only in specific conditions usually related to a perturbation of some kind of the boundary conditions at the surface of the substrate (see, e.g., [6]). Such conditions are for instance obtained by coupling with electric properties in piezoelectric materials of 6mm symmetry axis orthogonal to Π_S . These SAWs were discovered by Bleustein and Gulyaev in 1968. Their associated quasi-particles [1] and their perturbations are particularly easy to study in the present framework although coupling with quasi-electrostatics for dielectrics is necessary.

The standard solution of the BG surface wave is now well known via the introduction of an effective electric potential that accounts for the electromechanical coupling (cf. [7], Chapter 4). The corresponding point thermo-mechanics of the associated quasi-particle is obtained in the following Newtonian-Leibnizian form [1]:

$$\frac{d}{dt} P_{BG} = 0 , \quad \frac{d}{dt} K_{BG} = 0 , \quad (6)$$

wherein

$$P_{BG} := M_{BG} c_{BG} , \quad K_{BG} = \frac{1}{2} M_{BG} c_{BG}^2 , \quad (7)$$

$$M_{BG} = \frac{\rho_0 \pi U^2}{2 \bar{K}^2}$$

with

$$\bar{c}_T^2 = \bar{c}_{44} / \rho_0 , \quad \bar{c}_{44} = c_{44} (1 + K^2) , \quad (8)$$

$$K^2 = e_{15}^2 / \varepsilon_{11} c_{44} , \quad \bar{K}^2 = K^2 / (1 + K^2)$$

corresponding to the “dispersion” relation

$$D(\omega, k_1) := \omega^2 - c_{BG}^2 k_1^2 , \quad (9)$$

$$c_{BG} = \omega / k_{BG} = \sqrt{(\bar{c}_{44} / \rho_0) (1 - \bar{K}^4)}$$

In these equations, c_{44} , e_{15} and $\varepsilon_{11} = \varepsilon_0 + \chi_{11}$ are the only surviving elastic, piezoelectric and dielectric material coefficients for the 6mm symmetry. The results (6)-(7) are particularly simple with a momentum P_{BG} in the x_1 propagation direction, a mass M_{BG} that is naturally quadratic in the wave amplitude, and a quasi-particle kinetic energy K_{BG} that appears purely kinetic (via the mass M_{BG}) although originating in the continuum framework from kinetic, elastic, piezoelectric and electrostatic energies altogether. The BG solution (wavelike or particle-like) does not exist when the electromechanical coupling factor K vanishes.

3.2 Bleustein-Gulyaev SAWs perturbed by a weak elastic nonlinearity

The case where the volume energy of the above linear case is augmented by a small quartic elastic term to be treated further as a perturbation was recently treated in Ref.[8]. The physical system becomes a generator of *third harmonic*. In the treatment of the associated quasi-particle, the relevant representative domain of integration of the conservation equation is given by

$$\Omega = [0, \lambda_S] \times [0, +\infty) \times [0, 1] , \quad (10)$$

where $\lambda_S = 2\pi / k_S$ is the wavelength of the first harmonic component *as altered by the nonlinearity*. It is obtained that both the mass and the kinetic energy of the quasi-particle are increased compared to those of the linear case.

3.3 Bleustein-Gulyaev SAWs perturbed by a weak viscosity of the elastic substrate

This case is treated in detail in Ref. [9] to which the reader is referred. Both equations (2) and (3) acquire source terms in their right-hand sides. The

wavelike solution perturbed by an added small viscosity of the substrate is given in Ref.[10]. The quasi-particle motion becomes non-inertial with a source term due to friction. Simultaneously, the associated kinetic energy is no longer conserved. This case is distinctly remarkable in that the “mass” becomes a function of time and the associated quasi-particle momentum is no longer strictly parallel to the plane boundary: at order ε , the motion of our quasi-particle has become two-dimensional in the sagittal plane.

3.4 Murdoch SAWs

Another model that involves a unique SH displacement is the one introduced by Murdoch [11]. This model is particularly interesting because (i) of its purely mechanical nature, and (ii) of its relative simplicity with a *dispersive monomode* of propagation only (thus much simpler than the *dispersive multimode* Love SAWs). The basic field equations are

$$\rho_0 \frac{\partial^2 u_i}{\partial t^2} = \frac{\partial}{\partial x_j} \sigma_{ji} \text{ for } x_2 > 0 ; \quad (11)$$

$$\hat{\rho}_0 \frac{\partial^2 \hat{u}_i}{\partial t^2} = \frac{\partial}{\partial \hat{x}_j} \hat{\sigma}_{ji} - n_j \sigma_{ji}^+ \text{ at } x_2 = 0 . \quad (12)$$

Region $x_2 < 0$ is considered a vacuum. Here superimposed carets refer to quantities related to the surface of unit outward oriented normal n_j .

Thus $\hat{\sigma}_{ji}$ is a surface stress while $\sigma_{ji}^+ = \lim_{x_2 \rightarrow 0^+} \sigma_{ji}$ is the three-dimensional stress from the body. Mass density $\hat{\rho}_0$ is per unit surface, so that the limiting surface is endowed both with inertia and elasticity; it is a “material” surface. System (11)-(12) admits a pure SH SAW solution. We note

$$c_T^2 = \frac{\mu}{\rho_0}, \hat{c}_T^2 = \frac{\hat{\mu}}{\hat{\rho}_0}, k_a = \frac{\mu}{\hat{\mu}} . \quad (13)$$

The resulting SH SAW solution u_3 of (11)-(12) has a (true) dispersion relation given by

$$D(\omega, k_1) := \omega^2 - c_T^2 \left(k_1^2 - \frac{1}{k_a^2} \left(\frac{\omega^2}{\hat{c}_T^2} - k_1^2 \right)^2 \right) = 0, \quad (14)$$

and the solution exists only for phase velocities c such that $\hat{c}_T < c = c_M < c_T$.

It is shown that the canonical conservation laws of wave momentum and energy are obtained by combining those associated with the surface motion at $x_2 = 0$ with the volume ones integrated over the

depth in the substrate. The final result is a quasi-particle with Newtonian-Leibnizian properties, i.e.,

$$\frac{d}{dt} (M_M c_M) = 0, \quad \frac{d}{dt} \left(\frac{1}{2} M_M c_M^2 \right) = 0 \quad (15)$$

with mass given by

$$M_M = \left(\hat{\rho}_0 + \frac{\rho_0}{2\alpha} \right) U^2 \pi k_M, \quad (16)$$

$$k_M = k_1 = 2\pi / \lambda_M .$$

Here, α is the attenuation coefficient in depth such that

$$\alpha = \left(\frac{c^2}{\hat{c}_T^2} - 1 \right) \frac{k_1^2}{k_a}, \quad (17)$$

hence also a function of the wavelength. This provides an original example of quasi-particle associated with a *dispersive* SAW.

4 Transmission-reflection problem

4.1 Perfect interface between two solids

For the sake of simplicity we discard the attenuation in depth of the wave and thus consider a propagating SH face wave. Propagation from left (medium 1) to right (medium 2) is described by the equations of 1D linear elasticity in media 1 and 2 (respectively, with displacements u_1 and u_2) with matching conditions

$$u_1 = u_2, \quad \mu_1 u_{1,x} = \mu_2 u_{2,x} \text{ at } x=0. \quad (18)$$

and general solution in media 1 and 2

$$u_1 = u_I + u_R, \quad u_2 = u_T \quad (19)$$

with

$$\begin{aligned} u_1 &= U \cos(k_1 x - \omega t) + R_0 U \cos(k_1 x + \omega t), \\ u_2 &= T_0 U \cos(k_2 x - \omega t) \end{aligned} \quad (20)$$

where subscripts I , R and T refer to the incident, reflected and transmitted signals, respectively. The conservation of energy flux stands in the well known form

$$F_0 = 1 - R_0^2 - (z_2/z_1) T_0^2 \equiv 0. \quad (21)$$

where R_0 and T_0 are the reflection and transmission coefficients such that

($z_\alpha = \rho_\alpha c_\alpha$, $\alpha = 1, 2$, are impedances)

$$R_0 = \frac{z_1 - z_2}{z_1 + z_2}, \quad T_0 = \frac{2z_1}{z_1 + z_2}. \quad (22)$$

In the associated quasi-particle picture the local conservation laws of wave momentum and energy read in each medium

$$\frac{\partial H}{\partial t} - \frac{\partial Q}{\partial x} = 0, \quad \frac{\partial P}{\partial t} - \frac{\partial b}{\partial x} = 0, \quad (23)$$

where the energy or Hamiltonian per unit volume H , the energy flux Q , the wave momentum P and the (here reduced to a scalar) Eshelby stress b are defined by

$$H = \frac{1}{2} \rho u_t^2 + \frac{1}{2} \mu u_x^2, \quad Q = \sigma u_t = \mu u_x u_t, \quad (24)$$

$$P = -\rho u_x u, \quad b = -(L + \sigma u_x), \quad (25)$$

$$L = H - \sigma u_x$$

With the perfect interface at $x=0$, we can associate one quasi-particle with each wave component of the problem. With an obvious notation we have the following “masses”:

$$M_I = \rho_1 k_1 \pi U^2, \quad M_R = \rho_1 k_1 \pi R_0^2 U^2, \quad (26)$$

$$M_T = \rho_2 k_2 \pi T_0^2 U^2$$

The corresponding averaged wave momenta are given by

$$\bar{P}_I \equiv \langle P_I \rangle = \rho_1 \omega \pi U^2, \quad (27)$$

$$\bar{P}_R \equiv \langle P_R \rangle = -\rho_1 \omega \pi R_0^2 U^2, \quad (28)$$

$$\bar{P}_T \equiv \langle P_T \rangle = \rho_2 \omega \pi T_0^2 U^2$$

where we account for the fact that the averaged wave momentum \bar{P}_R is oriented towards negative x 's. We note ΔM , $\Delta \bar{P}$, and $\Delta \bar{H}$ the possible misfits in mass, momentum and kinetic quasi-particle kinetic energy defined by

$$\Delta M := (M_R + M_T) - M_I, \quad (29)$$

$$\Delta \bar{P} = (|\bar{P}_R| + |\bar{P}_T|) - |\bar{P}_I| \quad (30)$$

$$\Delta \bar{H} = (\bar{H}_R + \bar{H}_T) - \bar{H}_I \quad (31)$$

where the symbolism $|\dots|$ refers to the absolute value of its enclosure. That is, we are comparing the strengths of the momenta. We say that a quantity is conserved during the transmission-reflection problem if the corresponding misfit vanishes. It is shown that

$$\Delta \bar{H} = \left(\frac{1}{2} z_1 \omega \pi U^2\right) F_0, \quad (32)$$

where F_0 has been defined in (21). But the latter vanishes. Accordingly, $\Delta \bar{H} \equiv 0$: kinetic energy is

conserved in the transmission-reflection problem seen as a quasi-particle process that may be qualified of Leibnizian (conservation of *vis-viva*). But “mass” and momentum are not generally conserved in the present problem as it is immediately shown that

$$\Delta M = \rho_2 k_2 \pi T_0^2 U^2 \left(\frac{c_1^2 - c_2^2}{c_1^2} \right), \quad (33)$$

$$\Delta \bar{P} = \left(\frac{c_1 c_2}{c_1 + c_2} \right) \Delta M, \quad (34)$$

so that $\Delta \bar{P}$ and ΔM always are in the same sign. In particular, $\Delta M > 0$ if $c_1 > c_2$ and $\Delta M < 0$ if $c_1 < c_2$; $\Delta M = 0$ if and only if $c_1 = c_2$,

4.2 Imperfect interface with possible delamination

In the case of an *imperfect interface with possible delamination* where the matching conditions (18) are replaced by the conditions (known as Jones' conditions [12])

$$\sigma_1 = \sigma_2 \equiv K[u], \quad (35)$$

where K is a positive (spring) coefficient characterizing the degree of delamination and the symbol $[.]$ means the jump of its enclosure, i.e., $[u] = u_2 - u_1$ at $x=0$. We must look for *complex* solutions of the type $u = A \exp(i(kx - \omega t))$. Conditions (35) yield the following equation that replaces (21) – now $|R|$ and $|T|$ are the moduli of complex reflection and transmission coefficients:

$$F_K = 1 - |R|^2 - (z_2 / z_1) |T|^2 \equiv 0. \quad (36)$$

It is shown that

$$F_K = F_0 \left(1 - \frac{z_1^2 z_2^2}{z_1^2 z_2^2 + (K/\omega)^2 (z_1 + z_2)^2} \right). \quad (37)$$

The solution of this imperfect interface case is characterized by the parameter K/ω which shows the role played by the frequency ω . The limit case $K \rightarrow \infty$ corresponds to the *perfect interface* for which (21) holds true. The limit case $K \rightarrow 0$ corresponds to *full delamination* (no more transmission and complete reflection: $T=0$, $R=1$).

In the *associated quasi-particle picture*, there is no need to redo the computations. It suffices to

replace the transmission and reflection coefficients of the perfect case by the moduli of the new complex coefficients. Thus (32) is replaced by

$$\Delta \bar{H} = \left(\frac{1}{2} z_1 \omega \pi U^2 \right) F_K. \quad (38)$$

But this also vanishes by virtue of (36). Similarly, (33) holds with T_0^2 replaced by $|T|^2$ while (34) remains unchanged, noting that the coefficient $c_1 c_2 / (c_1 + c_2)$ does not depend on K . In the case when $K \neq 0$ but media 2 and 1 are identical, the presence of the K spring distribution can simulate a homogeneous surface of damage. In this case, both ΔM and $\Delta \bar{P}$ vanish so that K is no longer involved. The dependence on K shows only through the value of any of M_R, M_T, \bar{P}_R and \bar{P}_T .

4.3 Case of a sandwiched slab

In the case where an elastic slab (medium 2) of thickness d is sandwiched between two media of elastic type 1, the propagation considered is from left to right with reflection coefficient R in the left medium 1 and transmission coefficient T in the right medium 1. We assume that $d \gg \lambda_2$, where λ_2 is the (elastic wave) characteristic wavelength of medium 2, so that the association of quasi-particle properties makes sense in the slab. We need not reconsider the wavelike solution. It suffices to apply the results of the foregoing paragraphs to the two interfaces at $x=0$ (transition $1 \rightarrow 2$) and at $x=d$ (transition $2 \rightarrow 1$). Results are not reproduced here for lack of space.

In the case where we reduce the thickness d to zero while keeping the ratio μ_2/d finite the studied case reduces to the imperfect case of the previous paragraph with the surface elasticity coefficient $K = \mu_2/d$.

4.4 Case of a sandwiched multi-layer structure

With a careful bookkeeping, the formalism and "algebra" just introduced can be applied to the more complicated case where the sandwiched slab is made of a number $n-1$ of perfectly elastic layers (each with its own elastic properties) numbered $i=2, \dots, n$, all in perfect contact.

5 Concluding remark

The wealth of treated cases shows that the association of the waves of interest with the notion of quasi-particle is not a conceptually difficult

matter but it is limited by the analytical difficulties met in solving the wavelike continuum problem.

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