The tensor of interaction of a two-level system with an arbitrary strain field

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Abstract. The interaction between two-level systems (TLS) and strain fields in a solid is contained in the diagonal matrix element of the interaction hamiltonian, $\delta$, which, in general, has the expression $\delta = 2[\gamma] : [S]$, with the tensor $[\gamma]$ describing the TLS “deformability” and $[S]$ being the symmetric strain tensor. We construct $[\gamma]$ on very general grounds, by associating to the TLS two objects: a direction, $\hat{t}$, and a forth rank tensor of coupling constants, $[[R]]$. Based on the method of construction and on the invariance of the expression of $\delta$ with respect to the symmetry transformation of the solid, we conclude that $[[R]]$ has the same structure as the tensor of stiffness constants, $[[c]]$, from elasticity theory. In particular, if the solid is isotropic, $[[R]]$ has only two independent parameters, which are the equivalent of the Lamé constants. Employing this model we calculate the absorption and emission rates of phonons on TLSs and show that in isotropic solids, on average, the longitudinal phonons interact stronger with the TLSs than the transversal ones, as it is observed in experiments. We also show that in isotropic solids, a transversal wave leaves unperturbed all the TLSs with the direction contained in one of the two planes that are perpendicular either to the wave propagation direction or to the polarization direction and that a longitudinal strain applied to the solid polarises the TLS ensemble.

In a temperature range around ten Kelvins or below, the physical properties of amorphous materials differ significantly from the properties of crystals and show striking universal features (see [1] for a collection of reviews). Most of these features can be explained by assuming that in the amorphous solid exists a collection of dynamic defects, which are atoms or groups of atoms, oscillating in two well potentials. At low temperatures the thermal activation is suppressed and the oscillation happens by quantum tunnelling from one potential minimum to the other, forming in this way what is called a two-level system (TLS). In the two-dimensional Hilbert space spanned by the ground states of the two wells, the effective Hamiltonian of the TLS is

$$H_{TLS} = \frac{\Delta}{2} \sigma_z - \frac{\Lambda}{2} \sigma_x \equiv \frac{1}{2} \begin{pmatrix} \Delta & -\Lambda \\ -\Lambda & -\Delta \end{pmatrix}$$

(1)

where $\sigma_x$ and $\sigma_z$ are Pauli matrices, while $\Delta$ and $\Lambda$ are called the asymmetry of the potential and the tunnel splitting, respectively. The Hamiltonian (1) may be diagonalized by an orthogonal
transformation $O$, $H_{TLS}' \equiv O^T H_{TLS} O = \frac{1}{2} \sigma_z$, to obtain the excitation energy of the TLS, 
$\epsilon \equiv \sqrt{\Delta^2 + \Lambda^2}$—by the superscript $T$ we denote in general the transpose of a matrix. The parameters $\Delta$ and $\Lambda$ do not have the same values for all the TLSs, but are distributed with the density $V P(\Delta, \Lambda)$, where $V$ is the volume of the solid. According to the standard tunneling model (STM), this distribution is $P(\Delta, \Lambda) = P_0 / \Lambda$, with $P_0$ a constant. If expressed through the variables $\epsilon$ and $u \equiv \Lambda / \epsilon$, the distribution function becomes $P(\epsilon, u) = P_0 / (u\sqrt{1 - u^2})$.

A phonon, or any other strain in the solid body, perturbs $H_{TLS}$ by $H_1 \equiv (\delta / 2) \sigma_z$ [1; 2; 3; 4; 5]: The perturbation $\delta$ is linear in the strain field, $S_{ij}$, [1; 5] and in general may be written as $\delta \equiv 2 \gamma_{ij} S_{ij}$—here, as everywhere in this paper, we assume summation over repeated indices. The $3 \times 3$ symmetric strain tensor is defined as $S_{ij} = \frac{1}{2} (\partial_i u_j + \partial_j u_i)$, with $u_i \ (i = 1, 2, 3)$ being the components of the displacement field. In dyadic notations, $\delta = 2 [\gamma] : [S]$, where by $[\cdot]$ we shall denote matrices or second rank tensors.

In the construction of $[\gamma]$ we have to be more careful. In the STM, if $H_1$ is used to describe the interaction of TLS with phonons in three-dimensional (3D) bulk systems, the tensor $[\gamma]$ is replaced by a scalar, $\gamma_l$ or $\gamma_t$, depending whether the phonon has longitudinal or transversal polarization, respectively, while $S$ takes the value of the amplitude of the strain field. So one would write $\delta = 2 (\gamma_l S_l + \gamma_t S_t)$.

This picture cannot be applied to the interaction of TLS with arbitrary strain fields, at least because simple coordinate transformations may lead to ambiguity. It is well known from elasticity theory that by coordinate transformations longitudinal stress can be transformed into shear stress and vice-versa. To avoid this ambiguity, we have to keep $\gamma$ in the form of a tensor, not a simple matrix, and try to find its components [6]. So, the question we ask ourselves is how can we extract, on very general grounds, the tensor of interaction constants from the physical characteristics of the TLS—note that a tensor changes its components at the coordinate transformations while the value of $\delta$ should be the same in any coordinate system. Where can we begin to construct such a tensor?

Following the line of arguments from [6], we start by noting that since the TLS is represented as a tunneling entity between two potential wells—the transition from one classical equilibrium position to the other taking place either by a rotation or by a translation—we may associate to the TLS a direction in space, $\hat{t}$. So we have now three components, $t_1$, $t_2$, $t_3$, which change under coordinates transformations. The simplest $3 \times 3$ symmetric tensor that we can construct from $\hat{t}$ is $[T] = \hat{t} \cdot \hat{t}^T \ (T_{ij} = t_i t_j)$, while a general one would have the components $\gamma_{kl} \equiv R_{ij kl} T_{ij}$. In abbreviated subscript notations (see for example [7] for details), $T = (t^2_{xx}, t^2_{yy}, t^2_{zz}, 2t_{xy}, 2t_{xz}, 2t_{yz})^T$, and $R_{ijkl}$ becomes $R_{ij}$ in a straightforward way; in these notations $[\gamma]$ becomes the vector $\gamma \equiv [R]^T \cdot T$. Since $[S]$ is also transformed into $S \equiv (S_{xx}, S_{yy}, S_{zz}, 2S_{xy}, 2S_{xz}, 2S_{yz})^T$, the component of the interaction hamiltonian, $\delta$, is written simply as $\delta \equiv 2 \gamma_{ij} S_{ij}$, which, we say it again, is a scalar under coordinates transformations.

Now notice the analogy between $\delta$ and the elastic energy density, $u$, that exists in a deformed body. In abbreviated subscript notations, $u = \frac{1}{2} S^{ij} [c] \cdot S$, where $[c]$ is the $6 \times 6$ matrix of the elastic stiffness constants. Under a coordinate transformation, $S$ transforms into $S' = [N] \cdot S$, where $[N]$ is the $6 \times 6$ matrix of the transformation (see Ref. [7], Eq. 3.34), so

$$u = u' = \frac{1}{2} (S')^T \cdot [c] \cdot S' = \frac{1}{2} S^{T} \cdot [N]^T \cdot [c] \cdot [N] \cdot S.$$  

Since [2] should be valid for any $S$ and any transformation, then $[c]$ should remain unchanged—$[c] = [N]^T \cdot [c] \cdot [N]$—under the symmetry transformations of the crystalline lattice. From this argument follow all the properties of the matrix $[c]$ which are characteristic to the symmetries of the crystal under consideration [3].

The same is true for $\delta$. Here $T$ transforms in the same way as $S$ under coordinates transformations—$T' = [N] \cdot T$. Therefore $\delta \equiv \delta' = T^T \cdot [N]^T \cdot [R] \cdot [N] \cdot S$ and, like for $[c]$,
we have \([R] = [N]^T \cdot [R] \cdot [N]\) for any symmetry transformation \([N]\). In conclusion, \([R]\) has the same structure as the tensor of elastic stiffness constants (see also \(\boxed{3}\)).

If a material is isotropic, \([c]\) has only two independent parameters—the Lamé constants, \(\lambda\) and \(\mu\): \(c_{1IJ} = 2\mu \delta_{IJ} + \lambda\) for \(I, J \leq 3\) and \(c_{1IJ} = \delta_{IJ} \mu\) for \(I\) or \(J\) bigger than 3. In normal subscripts \(c_{ijkl}\) can be written in the more compact form, \(c_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})\). Based on the arguments above, the same is true for \([R]\); let us denote the independent parameters of \([R]\) by \(\zeta\) and \(\xi\), and, in normal subscripts, \(R_{ijkl} = \zeta \delta_{ij} \delta_{kl} + \xi(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})\). For a more straightforward reference to the STM, it might be even more convenient to denote \(\tilde{\gamma} = \xi + 2\tilde{\xi} \) and introduce the reduced tensor \(=[[r]]\) by \(r_{ijkl} \equiv R_{ijkl} / \tilde{\gamma} = \xi \delta_{ij} \delta_{kl} + \xi^t(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})\), where \(\xi^t = 2\xi' + 1\).

Using such a form of the coupling constants tensor, we calculated in \(\boxed{3}\) the scattering rate of phonons on the TLSs and showed that we recover the results of the STM after we average over the directions of the TLS, assuming that they are isotropically oriented. The two constants of the STM, \(\gamma_t\) and \(\gamma_{L}\), are related to the parameters in this model by \(\gamma_t = \gamma C_t\) and \(\gamma_{L} = \gamma C_{L}\), with

\[
C_t = \frac{1}{15}(15 - 40\xi' + 32(\xi')^2) \quad \text{and} \quad C_{L} = \frac{4}{15}(\xi')^2.
\]

From Eqs. \(\boxed{3}\) we see immediately that \(C_t > C_{L} \geq 0\) for any real \(\xi\), as it is observed experimentally in general \(\boxed{3}\).

What is also interesting to note, is that by calculating \(\gamma_t\) and \(\gamma_{L}\) from the experimental data, we can calculate \(\xi\) and \(\xi'\) and determine completely the tensor of coupling constants, \([R]\). For example the two different sets of values for \(P_0\gamma_t\) and \(P_0\gamma_{L}\) in fused silica, reported by Golding et al \(\boxed{8}\) (\(P_0\gamma_t^2 = 1.4 \times 10^{-5} \text{ J/m}^3\) and \(P_0\gamma_{L}^2 = 0.63 \times 10^{-5} \text{ J/m}^3\)) and Hunklinger and Arnold \(\boxed{9}\) (\(P_0\gamma_t^2 = 2.0 \times 10^{-5} \text{ J/m}^3\) and \(P_0\gamma_{L}^2 = 0.89 \times 10^{-5} \text{ J/m}^3\)), cited also by Black \(\boxed{10}\), give the same solutions for \(\xi'\): \(\xi_1' = 0.55\) and \(\xi_2' = 1.2\).

If we now go back to the interaction of a single TLS with a strain field and we assume that a transversal wave of strain field \(S = (0, 0, 0, S, 0, 0)^T\), is propagating through the solid, we find \(\delta = 2\tilde{\gamma} t_2 S t_2\). This means that any TLS of \(t_y = 0\) or \(t_z = 0\) (i.e. any TLS which is contained in a plane perpendicular either to the propagation direction or to the polarization direction) will not be perturbed by this wave.

Observing that for both values of \(\xi'\) calculated above, the corresponding values of \(\tilde{\zeta}'(= 1 - 2\xi')\) are negative, we show an interesting polarization effect of the TLS ensemble, due to an external stress. Let us assume that we apply a longitudinal stress along the \(z\) direction, \(S = (0, 0, S, 0, 0, 0)^T\). This stress gives a perturbation \(\delta = 2\tilde{\gamma} t_2^2 S t_2^2 + 2\tilde{\zeta}'(t_2^2 + t_2^2)\) and we notice that the two terms in the expression of \(\delta - \delta_1 = 2\tilde{\gamma} t_2^2 S t_2^2\) and \(\delta_1 = 2\theta_1(\tilde{\gamma} t_2^2 + t_2^2)\) have opposite signs. This means that, if e.g. \(\tilde{\gamma} t_2^2 S > 0\), the energy splitting, and therefore the excitation energy, of the TLSs oriented along the strain increase, while the energy splitting and the excitation energy of the TLSs oriented perpendicular to the strain direction decrease. In other words, the strain polarises the TLS ensemble.

In conclusion, we used a model for the interaction of two-level systems (TLS) with arbitrary strain fields, introduced in \(\boxed{3}\), which assumes that to any TLS is associated a direction, \(t\), and a tensor of coupling constants to the strain field, \([[R]]\), and we showed on general grounds that \([[R]]\) has the same structure with respect to the symmetry transformations of the solid as the tensor of stiffness constants, \([[c]]\), from the elasticity theory. Some immediate consequences of this formalism are that in isotropic solids, on average, the longitudinal phonons interact stronger with the TLSs than the transversal ones, \((\gamma_t > \gamma_{L}\) in the language of the standard tunnelling model), a transversal wave does not interact with the TLSs contained in one of the two planes that are perpendicular either to the wave propagation direction or to the polarization direction, and a strain applied to the body may polarize the TLS ensemble.
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