ON THE RELAXATION TIME OF CERTAIN TWO-LEVEL SYSTEMS IN AMORPHOUS STRUCTURES

L. Ferrari, G. Russo

To cite this version:


HAL Id: jpa-00220866
https://hal.archives-ouvertes.fr/jpa-00220866
Submitted on 1 Jan 1981

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
ON THE RELAXATION TIME OF CERTAIN TWO-LEVEL SYSTEMS IN AMORPHOUS STRUCTURES

L. Ferrari and G. Russo*

Istituto di Matematica dell'Universitá - Ferrara, Italy
Gruppo Nazionale di Struttura della Materia - Unità di Bologna - Bologna, Italy
* Istituto di Fisica dell'Universitá - Bologna, Italy
Gruppo Nazionale di Struttura della Materia - Unità di Bologna - Bologna, Italy

Abstract. The origin and dynamics of 2-level systems in amorphous structures have been recently interpreted by the authors in terms of D-D intimate pairs interactions. Since the "tunnelling" particles are electrons (and not atoms) and the quantum picture of the model is quite different from that first introduced by Anderson et Al. in 1972, the problem concerned with the relaxation time $\tau$ of 2-level systems has been reviewed and re-calculated. At given temperature, $\tau$ is shown to be much shorter than predicted by previous theories. It is suggested that the corresponding 2-level systems represent the "anomalous" (or fast) ones introduced by Black and Halperin for interpreting some time-dependent experimental data obtained at low temperature.

Introduction. The relaxation time $\tau$ is a quantity directly related to the detailed structure of the 2-level systems present in many amorphous substances, hence the relevance of $\tau$ for getting reliable information about the origin of 2-level systems themselves has increased more and more in recent years (1) giving rise, among other things, to some challenging questions whose clearest example is the dependence of some thermodynamical quantities on the measurement time (1,2).

In a recent, still unpublished paper ("Charged dangling bonds and two-level systems in amorphous solids") the authors have developed a model for the 2-level systems dynamics which strongly differs from the previous ones especially as far as the nature of the defects corresponding to the 2-level systems is concerned.

The model deals with D-D (opposite charged dangling bonds) intimate pairs, forming electric dipoles whose allowed "motion" at low temperature, is simply a charge interchange; it is suggested (3) that a certain percentage of such defects is formed at the surface of some crystalline inclusions characteristic of many amorphous substances (4). Finally it has been shown that crystalline inclusions containing 2 electric dipoles may give origine to 2-level systems due to dipole-dipole interactions. Behind the complicated details of the model, a clear dynamical feature is remarkable even at a first sight: the "moving" particles are no longer atoms or groups of atoms, but, if any, pairs of electrons. The second remark is that the defect cannot be described in terms of a double potential well scheme, as Anderson et Al. did in 1972 (5); in the present model, in fact, 2-level systems are originated by a rather complicated coupling between charged defects, so that the calculation of $\tau$ requires a different and subtler dynamical picture.

The basic formula one is concerned with is the standard one, essentially derived from Fermi's Golden Rule (6):
where $V$ is the perturbing potential due to the elastic strain, $|1\rangle$ and $|2\rangle$ are quantum states corresponding to the 2-level systems separated by the energy splitting $E$, and $C$ is given in terms of the sound velocities $C_s$ and $C_t$ as follows:

$$C^{-5} = C_{1s}^{-5} + 2C_{ts}^{-5}.$$  

In expression (1) the detailed structure of the 2-level systems is contained in the matrix element $\langle 1|V|2\rangle$. In the model under consideration the energy quantum $E$ is gained (or lost) when one dipole is at rest (and, say, upward directed) while the second dipole "switches up" from the downward position (or vice-versa). Hence, apart from very complicated but negligible deformation effects, the whole 2-dipole system can be approximately described in terms of the wave functions corresponding to the "switching" dipole only and hence one assumes, according to a chemical-physical picture of weak polar bonds:

$$|1\rangle = \frac{|a\rangle + |b\rangle}{(a^2 + 1)^{1/2}},$$

$$|2\rangle = \frac{|b\rangle - |a\rangle}{(a^2 + 1)^{1/2}}.$$  

where $|a\rangle$ and $|b\rangle$ are bi-electronic normalised wave functions representing $D$ in each of the two atomic sites $a$ and $b$ where the $D$ $D$ pair is located. Orthogonality of $|1\rangle$ and $|2\rangle$ is given by the assumption:

$$\langle a|b\rangle \ll 1.$$  

The real parameter $\alpha$ is related to the dipole momentum $M$ of the electric dipole according to the formula:

$$M = e\langle 1|\vec{r}|1\rangle = e\langle 2|\vec{r}|2\rangle.$$  

Assuming that:

$$\langle a|\vec{r}|a\rangle = \frac{R}{2},$$

$$\langle b|\vec{r}|b\rangle = -\frac{R}{2}$$ and

$$|\langle a|\vec{r}|b\rangle| \ll R,$$

expression (3) can be used for determining $\alpha$ as a function of $M$ and $R$ (the distance between the atomic sites $a$ and $b$). The value of $M$ can be determined from experiments (7) and, for $a$-$SiO_2$, it turns out to be
On the contrary, an estimate for $R$ is rather difficult although its value ranges, according to the origin of the model (4), between 1 and $10^9$. Hence an average value of $4.55 \times 10^7$ seems to be reliable and thus, from rel.s (4), (3) and (2), one has

\[ a^2 = \frac{eR-2M}{eR+2M} \approx 0.6 \quad (5) \]

According to a standard procedure (6), one now assumes that $V$ is diagonal in the $|a>$ and $|b>$ basis; then a straightforward calculation gives (6):

\[ |<1|V|2>| = \frac{\alpha B}{a^2+1} \quad (6) \]

where $B$ is the deformation potential with a rough magnitude of 1 eV. Thus from formulas (1), (4), (5) and (6), one finally obtains:

\[ \tau^{-1} = \frac{2^2 \alpha^3 E^3}{c5(a^2+1)^22\pi qH^4} \coth(E/2K_BT) \quad (7) \]

Expression (7) shows that the relaxation time deduced from the dipolar model, for given $T$ and $E=K_BT$ is comparable with the lowest value among the ones predicted by theories based on tunnelling atoms (2,5). Hence the conjecture that the dipolar 2-level systems can correspond to the "anomalous" (or fast) ones proposed by Black and Halperin (8) for explaining some time-dependent experimental data (9), seems to be very reasonable. This conjecture has been tested according to data deduced from ref. (1) (see in particular pag. 41). It has been found that at $T=0.16K$, the relaxation time for processes involving 2-level systems strongly coupled with the dominant phonon is about $10^{-5}$ sec, in excellent agreement with the expected value for the "anomalous" levels, as given in ref. (1) (pag. 41). Furthermore it is noticeable that "anomalous" levels have been introduced without increasing the value of $B$; thus it is likely that the present model can overcome the difficulties connected with a too strong coupling of "anomalous" 2-level systems with phonons. Finally, the relation among 2-level systems and electric dipoles, supported by experimental evidence (7), clearly reflects on the relaxation time through parameter $\alpha^2$; using rel. (5) it is possible to re-write the expression for $\tau^{-1}$ as follows:

\[ \tau^{-1}(M,E) = \left[ 1 - \left( \frac{2M}{eR} \right)^2 \right] \frac{B^2E^3}{c^58\pi qH^4} \coth(E/2K_BT) \quad (8) \]

where the dependence of $\tau$ on $M$ has been made explicit.
References:
(1) "Amorphous Solids" (Low-Temperature Properties); Editor: W.A. Phillips, SPRINGER-VERLAG - Berlin (1981)
(2) J. L. Black; Phys. Rev. B 17 No6, 2740 (1978)
(3) L. Ferrari and G. Russo; Lett. N. Cim. 30 No6, 184 (1981)
(5) P.W. Anderson, B. I. Halperin and C.M. Varma; Phil. Mag. 25, 1 (1972)
(6) J. Jackle; Z. Physik 257, 212 (1972)
(9) W.M. Gobau and R.M. Tait; Phys. Rev. Lett. 34, 1220 (1975)