LATTICE PHONON LIFETIME CALCULATIONS
J. Henkel

To cite this version:
J. Henkel. LATTICE PHONON LIFETIME CALCULATIONS. Journal de Physique Colloques, 1981, 42 (C6), pp.C6-146-C6-148. 10.1051/jphyscol:1981644. jpa-00221580

HAL Id: jpa-00221580
https://hal.science/jpa-00221580
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.
LATTICE PHONON LIFETIME CALCULATIONS

J.H. Henkel

Department of Physics and Astronomy, University of Georgia, Athens, Georgia 30602, U.S.A.

Abstract.—It is shown that phonon lifetimes can be calculated using finite periodicities and discrete frequencies without going completely to the limit of infinite periodicities or quasi-continuous frequency distributions. In applying the Golden Rule equation in time-dependent perturbation theory there is a time interval over which the transition rate is very nearly independent of time and energy level differences (or periodicity). As the periodicity of the lattice increases the time interval over which the transition rate is independent of time increases and approaches infinity in the limit of infinite periodicity. Calculations are presented.

The Golden Rule of time-dependent perturbation theory relating transition rates from an initial unperturbed energy eigenstate \( E_n(0) \) to one of the other energy eigenstates \( E_m(0) \) induced by the perturbing Hamiltonian \( H' \) with matrix elements \( H'_{mn} \) is given by

\[
w = \frac{1}{\hbar} \sum_m' |a_m(t)|^2 = \frac{2}{\hbar} \sum_m' |H'_{mn}|^2 \frac{1 - \cos \left( \frac{\omega_{mn} t}{\hbar} \right)}{\omega_{mn}^2},
\]

(1)

where

\[
\omega_{mn} = \frac{E_m(0) - E_n(0)}{\hbar}
\]

(2)

and where the prime on the sum means that the term for \( m = n \) is excluded from the sum. The Golden Rule can also be written as

\[
w = \frac{d}{dt} \sum_m' |a_m(t)|^2 = \frac{2}{\hbar} \sum_m' |H'_{mn}|^2 \frac{\sin \left( \frac{\omega_{mn} t}{\hbar} \right)}{\omega_{mn}}
\]

(3)

For quasi-continuous energy distributions the Golden Rule takes the form

\[
w = \frac{2\pi}{\hbar} |H'_{mn}|^2 \rho(E_n(0)),
\]

(4)

where \( \rho \) is the density of states expressed as a function of \( E_n(0) \) and where the right hand side is independent of time \( t \).

To see how phonon lifetimes can be calculated using the Golden Rule equation without first taking the limit of quasi-continuous energy
level distributions consider the functions $F_1(\alpha,t,L)$ and $F_2(\alpha,t,L)$ given by

$$F_1(\alpha,t,L) = \frac{2}{L} \sum_{n=1}^{L} \frac{\sin \frac{2\pi}{L}(\alpha - n)t}{\sin \frac{2\pi}{L}(\alpha - n)}$$

and

$$F_2(\alpha,t,L) = \frac{1}{L} \sum_{n=1}^{L} \frac{1 - \cos \frac{2\pi}{L}(\alpha - n)t}{\left(\frac{2\pi}{L}(\alpha - n)\right)^2}$$

In the limit $L \to \infty$ these functions are unity independent of time $t$ provided $0 < \alpha < L$ but not one of the integers 1, 2, ..., L. For finite $L$ the functions are to within about 10% equal to unity independent of $\alpha$ and $t$ for the interval $1 < t < L$ and for $0 < \alpha < L$ with $\alpha \neq 1, 2, ..., L$. A plot of a typical $F_1(\alpha,t,L)$ versus $t$ is shown in Fig. 1 while Table I lists calculated values of $F_1(\alpha,t,12)$. The function $F_1(\alpha,t,L)$ is zero at $t=0$, with a slope $\frac{dF_1(\alpha,0,L)}{dt} = 2$, and levels off to approximately 1 at $t=1$. It remains unity within small variations up to $t=L$ independent of $\alpha$ provided $0 < \alpha < L$ and $\alpha \neq 1, 2, ..., L$.

Two important conclusions result in examining the properties of $F_1(\alpha,t,L)$. One is that the value of $F_1(\alpha,t,L)$ for $1 < t < L$ is approximately the same as the limiting value of $F_1(\alpha,t,\infty)$. The other is that the convergence in $L$ is very rapid. The main result in increasing $L$ is the increase in time interval over which $F_1$ is constant.

The potential energy expression of a crystal can be expanded in series form involving the atomic displacements. That part of the potential including the third degree terms in the displacements can be used as the perturbing potential utilized in the Golden Rule equation to calculate time derivatives of phonon occupation densities. When this is done the derivative takes the following form

$$\frac{dn_{\sigma}}{dt} = \sum_{\sigma',\sigma''} 2 |C_{\sigma',\sigma'',\sigma}|^2 \frac{A}{M\omega'\omega''} \frac{\sin \Delta \omega t}{\Delta \omega} \times (n_{\sigma} + 1)n_{\sigma'} - n_{\sigma}(n_{\sigma'} + 1)(n_{\sigma''} + 1),$$

where

$$\Delta \omega = \omega_{\sigma} - \omega_{\sigma'} - \omega_{\sigma''}$$

This derivative can be evaluated for different times by direct summation of finite sums obtained using finite periodic boundary conditions. The above analysis of the properties of $F_1(\alpha,t,L)$ indicates that this derivative $\frac{dn_{\sigma}}{dt}$ using finite periodicity should be roughly constant over a time interval $\varepsilon < t < \frac{2\pi}{|\Delta \omega|_m}$, where $|\Delta \omega|_m$ is a minimum value of $|\Delta \omega| = |\omega_{\sigma} - \omega_{\sigma'} - \omega_{\sigma''}|$. The analysis also indicates that the convergence in $L$ should be very rapid and that the constant
value obtained should be within about 10% of the value obtained in the limit of infinite periodicity. An advantage of the use of finite periodic boundary conditions with the resulting finite sums is that the complex phase relations involving conservation of momentum and energy is automatically included in the sums.

![Plot of typical value of $F_1(a,t,L)$ versus $t$. Independent of $a$ for $0 < a < L$, $a \neq 1,2,\ldots,L$.]

**TABLE I.** Calculated values of $F_1(a,t,12)$

<table>
<thead>
<tr>
<th>$t$</th>
<th>3.1</th>
<th>3.2</th>
<th>3.3</th>
<th>3.4</th>
<th>6.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>.4</td>
<td>.68</td>
<td>.68</td>
<td>.68</td>
<td>.69</td>
<td>.73</td>
</tr>
<tr>
<td>.8</td>
<td>.89</td>
<td>.90</td>
<td>.92</td>
<td>.93</td>
<td>1.14</td>
</tr>
<tr>
<td>1.2</td>
<td>.91</td>
<td>.92</td>
<td>.93</td>
<td>.94</td>
<td>1.15</td>
</tr>
<tr>
<td>1.6</td>
<td>1.03</td>
<td>1.04</td>
<td>1.04</td>
<td>1.05</td>
<td>.98</td>
</tr>
<tr>
<td>2.0</td>
<td>1.12</td>
<td>1.12</td>
<td>1.12</td>
<td>1.12</td>
<td>.90</td>
</tr>
<tr>
<td>2.4</td>
<td>1.08</td>
<td>1.08</td>
<td>1.07</td>
<td>1.07</td>
<td>.96</td>
</tr>
<tr>
<td>2.8</td>
<td>1.06</td>
<td>1.05</td>
<td>1.04</td>
<td>1.03</td>
<td>1.06</td>
</tr>
<tr>
<td>6.0</td>
<td>1.02</td>
<td>1.04</td>
<td>1.06</td>
<td>1.07</td>
<td>.95</td>
</tr>
</tbody>
</table>

References: