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DEPARTAMENTO DE FÍSICA

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PONTIFÍCIA UNIVERSIDADE CATÓLICA DO RIO DE JANEIRO
DEPARTAMENTO DE FÍSICA
Rua Marquês de São Vicente, 225
Cx. Postal 38071 Telegramas FISPUC
22453 – Rio de Janeiro – Brasil

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ON THE MINIMA OF THE TIME INTEGRATED PERTURBATION FACTOR IN THE SCHERER-BLUME THEORY*

E.F. da Silveira and F.L. Freire Junior

Departamento de Física, Pontifícia Universidade Católica
Cx.P. 38071, Rio de Janeiro, RJ, Brasil

C.P. Massolo**

Institut de Physique Nucléaire, Orsay, France

F.A. Schaposnik**

Laboratoire de Physique Théorique et Hautes Energies***
Université Pierre et Marie Curie, Paris, France

A. Lépine

Instituto de Física, Universidade de São Paulo
Cx.P. 20916, Cidade Universitária, SP, Brasil

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ABSTRACT. The minima in the correlation time dependence of the Scherer-Blume time integrated attenuation coefficients for the hyperfine perturbation of ions recoiling in gas are studied. Its position and depth are determined for different physical situations and comparison with experimental data is shawn.

RESUMO. Estudamos os mínimos que aparecem na dependência com o tempo de correlação dos coeficientes de atenuação integrados com relação ao tempo fornecidos pela teoria de Scherer-Blume. Determinou-se suas posições e profundidades em diferentes situações físicas. Uma comparação com dados experimentais também é mostrada.

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** On leave of absence from Universidad Nacional de La Plata, Dep. of Phys., C.C. 67, La Plata, Argentina.

*** Laboratoire Associé au CNRS, France.

1. INTRODUCTION

Measurements of γ-γ angular correlations perturbed by hyperfine interactions experienced by excited nuclei recoiling in gas are used extensively for the determination of magnetic moments of nuclear levels [1], as well as for the investigation of the atomic processes involved [2]. The measured attenuation coefficients are usually compared with those evaluated using the theory developed by C. Scherer [3] and M. Blume [4] based on a stochastic perturbation model.

A striking feature in the behavior of the perturbation factor is the observed minimum in the correlation time dependence of the attenuation coefficients [1,2,7]. Remarcably enough, the existence of this minimum is predicted by the Scherer-Blume theory although its physical meaning remains obscure.

Some approximate conditions for the existence of the minimum have been derived by Zemel and Niv (5) for the correlation time dependence of the time differential coefficient ($G_K(t)$). They show that the position of the minimum is directly proportional to the g-factor of the nucleus and its depth is a function of the time the hyperfine fields acts on the nucleus.

The purpose of the present note is to study the dependence of the time integrated coefficient ($\overline{G_K}(\infty)$) with the correlation time in an attempt to gain some understanding about the influence of the atomic process involved in the recoiling of excited nuclei in gas. In particular, we focussed our attention of the properties of the minima of $\overline{G_K}(\infty)$, looking for existence conditions and simplified expressions describing its positions and depth.

2. RESULTS

Our starting point is the expression for the time integrated perturbation coefficients obtained by Blume [4]:

$$\overline{G_K}(\infty) = \left[\frac{1}{\sum_\nu \left[C_\nu/(1+\tau/\tau_c + i\omega_\nu\tau)\right]} - \frac{\tau}{\tau_c} \right]^{-1} \quad (1)$$

The frequencies ω_ν are given by $\omega_\nu \equiv \omega_{FF'} = (E_F - E_{F'})/\hbar$, where E_F and $E_{F'}$ are the eigenvalues of the hyperfine interactions Hamiltonian.

The coefficients C_ν are products of a geometrical term, depending on the atomic angular momentum J, the nuclear spin I, the total angular momentum F, and a statistical term specifying the charge state distribution and the probability of occupation of a certain configuration within this charge state [6]. They are real numbers satisfying

$$C_\nu = C_{-\nu} \qquad \text{and} \qquad \sum_\nu C_\nu = 1 \quad (2)$$

If we are looking for a minimum of $\overline{G_K}(\infty)$ when τ_c varies, we have to solve

$$\left. \frac{\partial \overline{G_K}(\infty)}{\partial \tau_c} \right|_{\tau_c = \tau_c^*} = 0 \quad (3)$$

where τ_c^*'s are the values of τ_c which minimize (1).

Using eqs. (1)-(3), we get

$$\sum_\nu \frac{C_\nu}{(1+\tau/\tau_c^* + i\omega_\nu\tau)^2} = \left[\sum_\nu \frac{C_\nu}{1 + \tau/\tau_c^* + i\omega_\nu\tau}\right]^2 \qquad (4)$$

We now introduce the "effective mean-life" τ_{eff}:

$$\frac{1}{\tau_{eff}} = \frac{1}{\tau} + \frac{1}{\tau_c} \qquad (5)$$

which, for "pure" static ($\tau << \tau_c$) interactions reduces to the nuclear mean life τ, thus controlling the position of the minimum. On the other hand for highly fluctuant hyperfine fields ($\tau >> \tau_c$), $\tau_{eff} \approx \tau_c$ and the correlation time dominates the behaviour of the perturbation factor.

Using the fact that $\omega_\nu = -\omega_{-\nu}$, we then obtain the following equation in terms of τ_{eff}:

$$C_0 + \sum_{\nu\neq 0} C_\nu \frac{1 - \omega_\nu^2 \tau_{eff}^{*2}}{[1 + \omega_\nu^2 \tau_{eff}^{*2}]^2} = \left\{C_0 + \sum_{\nu\neq 0} \frac{C_\nu}{1 + \omega_\nu^2 \tau_{eff}^{*2}}\right\}^2 \qquad (6)$$

The solutions of this equation give the values of $\tau_{eff} = \tau_{eff}^*$ (and consequently of τ_c^*) for which $\overline{G_K}(\infty)$ shows a minimum. We note that the solutions are not always real: for instance, when $\omega_\nu \tau_{eff} \leq 1$ for all positive ν, $\overline{G_K}(\infty)$ does not exhibit minima. It is not possible in general to find an analytical solutions of eq. (6) and therefore it will be useful to consider the following different situations:

i) systems with three hyperfine frequencies, one of which is zero and the other two equal in magnitude, but with opposite signs;

ii) systems with several frequencies very different from one another;

iii) systems where these frequencies are approximately the same.

i) <u>Only one frequency with modulus different from zero</u>

When there are only two possible values of F, one has necessarily $\omega_o = 0$ and $\omega_1 = -\omega_{-1} \equiv \omega$ and eq.(6) is easily solved, giving just one solution

$$\tau^*_{eff} = \frac{1}{\omega\sqrt{C_o}} \qquad (7)$$

or, in terms of the correlation time;

$$\tau^*_c = \frac{\tau}{\omega\tau\sqrt{C_o} - 1} \qquad (8)$$

Since τ^*_c must be positive, the condition for the existence of a minimum turns out to be $\omega\tau\sqrt{C_o} > 1$. Taking $\sqrt{C_o} \simeq 1$ (as it is usually the case) eq.(8) can be rewritten as:

$$\tau^*_c = \frac{\tau}{\omega\tau - 1} \qquad (9)$$

One can see that if $\omega\tau \gg 1$, i.e., on the average the nuclei precess several times before the de-excitation process takes place, then the following relation holds:

$$\tau^*_c = \frac{1}{\omega} \qquad (10)$$

Showing that the minimum of $\overline{G_K}(\infty)$ occurs when the frequency of atomic collisions coincides approximately with the hyperfine frequency.

We also note that in this situation the position of the minimum is not sensible to the probability of occupying states with different values of F.

Another relevant quantity is the minimum value of $\overline{G_K}(\infty)$. Substitution of eq.(8) into eq.(1) gives:

$$\overline{G_K}(\infty)\Big|_{\tau_c = \tau_c^*} = \left[1 + \frac{C_1}{\sqrt{C_o}}\,\omega\tau\right]^{-1} \qquad (11)$$

Eq.(11) shows that while the position of the minimum of $\overline{G_K}(\infty)$ depends uniquely on ω, the depth of this minimum is a function of the coefficient C_ν which are directly related to the cross sections of the atomic interactions involved. It will be seen below that the product $C_\nu\omega_\nu$ also plays an important role when several frequencies are present.

We can also note from eq.(11) that $\overline{G_K}(\infty)$ cannot be zero. This is simply a consequence of the fact that the nuclei are initially aligned and, irrespective how strong the perturbation is, the average-in-time alignment will never be exactly zero.

Fig. 1a shows the shape of the attenuation coefficients $\overline{G_2}(\infty)$, for this particular case, as a function of τ/τ_c for a set of relevant parameters.

ii) <u>Several frequencies: $|\omega_1| \gg |\omega_2| \gg |\omega_3| \ldots$</u>

Although an analytical solutions of (.) cannot be reached, numerical calculations of (1) for particular cases can show relevant features of the correlation time dependence of the attenuation coefficients. When all hyperfine frequencies involved are quite different from one another, numerical analysis shows the existence of several minima on $\overline{G_K}(\infty)$, each of them with characteristics roughly equal to those corresponding to a $\overline{G_K}(\infty)$ with just one specific frequency. In other words, the shape of $\overline{G_K}(\infty)$ corresponding to several frequencies can be approximately obtained by superposing the shapes of $\overline{G_K}(\infty)$'s corresponding to a single $|\omega_\nu|$.

Fig. 1b illustrates these features as well as the influence of the product $C_\nu \omega_\nu$ in the depth of each minimum.

iii) <u>Several frequencies with moduli quite near: $|\omega_1| \simeq |\omega_2| \simeq |\omega_3| \ldots$</u>

We will write in this case

$$\omega_\nu^2 = \omega_o^2 + \Delta(\omega_\nu^2) \qquad (12)$$

with the condition $\Delta(\omega_\nu^2) \ll \omega_o^2$.

Defining x_ν and ε_ν, $(\varepsilon_\nu \ll x_o)$:

$$x_\nu \equiv \omega_\nu^2 \tau_{eff} = \omega_o^2 \tau_{eff}^2 + \Delta(\omega_\nu^2)\tau_{eff}^2 \equiv x_o + \varepsilon_\nu \qquad (13)$$

it is possible to re-write eq.(6) as

$$C_o + \sum_{\nu\neq 0} C_\nu \frac{1-x_o}{(1+x_o)^2} \left(1 - \frac{\varepsilon_\nu}{1+x_o}\right)^2 \left(1 - \frac{\varepsilon_\nu}{1-x_o}\right) =$$

$$= \left\{ C_o + \sum_{\nu\neq 0} C_\nu \left(\frac{1}{1+x_o}\right) \left(\frac{1-\varepsilon_\nu}{1+x_o}\right) \right\} \qquad (14)$$

Neglecting terms of second order in the ε_ν expansion, assuming $x_o \neq 1$, and using (2), we get

$$x_o(1-x_o^2)(C_o x_o - 1) = \{1-x_o - 2\, C_o x_o (1+x_o)\}\bar{\varepsilon} \qquad (15)$$

where $\bar{\varepsilon} \equiv (\sum_{\nu\neq 0} C_\nu \varepsilon_\nu) / \sum_{\nu\neq 0} C_\nu$

An interesting simplification takes place if we choose $x_o = \bar{x} \equiv (\sum_{\nu\neq 0} C_\nu x_\nu)/\sum_{\nu\neq 0} C_\nu$ (i.e. $\omega_o^2 = \overline{\omega^2}$). In fact $\bar{\varepsilon}$ being equal to zero for this choice and being $x_o(1-x_o) \neq 1$, eq.(15) reduces to

$$C_o\, \tau_{eff}^2\, \overline{\omega^2} = 1 \qquad (16)$$

This equation is essentially equivalent to eq.(7) and like wise characterizes the presence of just one minimum. Using the notation $\bar{\omega} \equiv (\overline{\omega^2})^{1/2}$, and the conditions $C_o \simeq 1$ and $\tau >> \tau_c$, we finally have

$$\tau_c{}^* = \frac{1}{\bar{\omega}} \qquad (17)$$

Note that this equation is formally identical to eq.(10) (which corresponds to the case of only one non-zero frequency ω). The only change when several similar frequencies are present is that the average $\bar{\omega}$

appears instead of ω.

If $\omega_\nu \tau_{eff} \approx 1$ for all ν, the assumption $x_o \neq 1$ is not satisfied in (15). A similar derivation however gives $\tau^*_{eff} \overline{\omega^2} = 3/(2+C_o)$ and therefore, (17) remains unchanged.

The value of $\overline{G_K}(\infty)$ in the minimum can now be obtained by substituting of eq.(17) into eq.(1):

$$\overline{G_K}(\infty)\Big|_{\tau_c = \tau_c^*} = \left[1 + \frac{1 - C_c}{2\,C_o}\,\frac{\tau}{\tau^*_{eff}}\right]^{-1} = \left[1 + \frac{1 - C_o}{2\,\sqrt{C_o}}\,\bar{\omega}\,\tau\right]^{-1} \tag{18}$$

The similarity between equations (18) and (12) shows again that the effect on $\overline{G_K}(\infty)$ of several hyperfine frequencies, which are not quite different one from another, is equivalent to the effect of an average frequency $\bar{\omega}$.

Finally, it is interesting to note that eq.(18) can be alternatively obtained in the approximation $C_o \approx 1$ by taking the time average of $G_K(t,\tau_c^*)$ given in ref.[5].

3. DISCUSSION AND APPLICATIONS

The equation for $\overline{G_K}(\infty)$ which we have used, (eq.1), assumes that τ_c is mantained constant during the de-excitation of the nuclear state. Therefore to compare our results with experimental values we have to search look for a physical system satisfying this condition. An example is found in the decay of ^{127}Xe into ^{127}I in gaseous sources through the 203 KeV level (τ = 0.55 ns).

Fig. 2 shows a comparison between experimental data [7] and our theoretical results. The abcissa τ/τ_c was obtained taking $\tau_c = 1/nv\sigma$, where n is the number of molecules per cm^3, v is the thermal velocity of the ions ($2,5 \times 10^4$ cm/s) and σ is the total atomic cross sections ($808 \pm 234 \times 10^{-15}$ cm^2) [8]. Thus, the relation between τ_c and pressure for this case is $\tau_c(ns) = 1.4/P$ (torr).

Considering now the existence of only one minimum, at 60 torr, in the $\overline{G_2}(\infty)$ dependence with pressure, we can use the results obtained in section 2 to calculate C_o and $\bar{\omega}$. For the present purposes, these calculations were performed in the scope of just one frequency with modulus different from zero.

The obtained values are: $C_o = 0.22$ and $\bar{\omega} =$ 92.7 GHz, (which satisfy the condition $\omega\tau \sqrt{C_o} > 1$ for the existence of a minimum).

Using these values, one can now compute the theoretical $\overline{G_2}(\infty)$ which turns out to be in very good agreement with the experimental data *in the whole range* of τ_c.

Thus, our analysis shows that, although the Scherer-Blume stochastic model relies on a considerable amount of limitative assumptions, it nevertheless reproduces fairly well the actual experimental data in the whole range of τ_c.

Concerning the approximate expressions that we have obtained they have shown to be reasonably precise as to be employed in the study of fluctuating hyperfine fields when the presence of too many frequencies makes the use of the exact equation very "complicated". In particular, they provide a simple way of restricting the τ_c - region where the minimum of the attenuation coefficient occurs.

It is interesting to note that the approximate expressions given by eq.(10) and eq. (17) show that the experimental determination of the position of the minima gives the value of the hyperfine frequency $\omega(\bar{\omega})$ and hence the magnetic field acting on the nucleus. On the other hand, the knowledge of the depth of the minima provides information about the occupation probability of the atomic states.

As we stated above no satisfactory explanation of the existence of the minimum has been found. It is only known [9] that solely "fluctuating orientation" models reproduce this property of the attenuation factor which has been found experimentally. Although no general conclusion may be drawn from our computations, they indicate that the value of τ_c at which it occurs is directly related to an average of the hyperfine frequencies weighted with the coefficients C_ν, related to the charge state distribution and occupation probabilities of the hyperfine levels.

We end by noting that our computations show that for the case of several frequencies quite different from one another the existence of more than one minimum is to be expected in $\overline{G_2}(\infty)$. In this case (which, to our knowledge, has not been yet found experimentaly) the shape of the curve should be a superposition of $\overline{G_K}(\infty)$'s each one corresponding to a single hyperfine frequency ω_ν.

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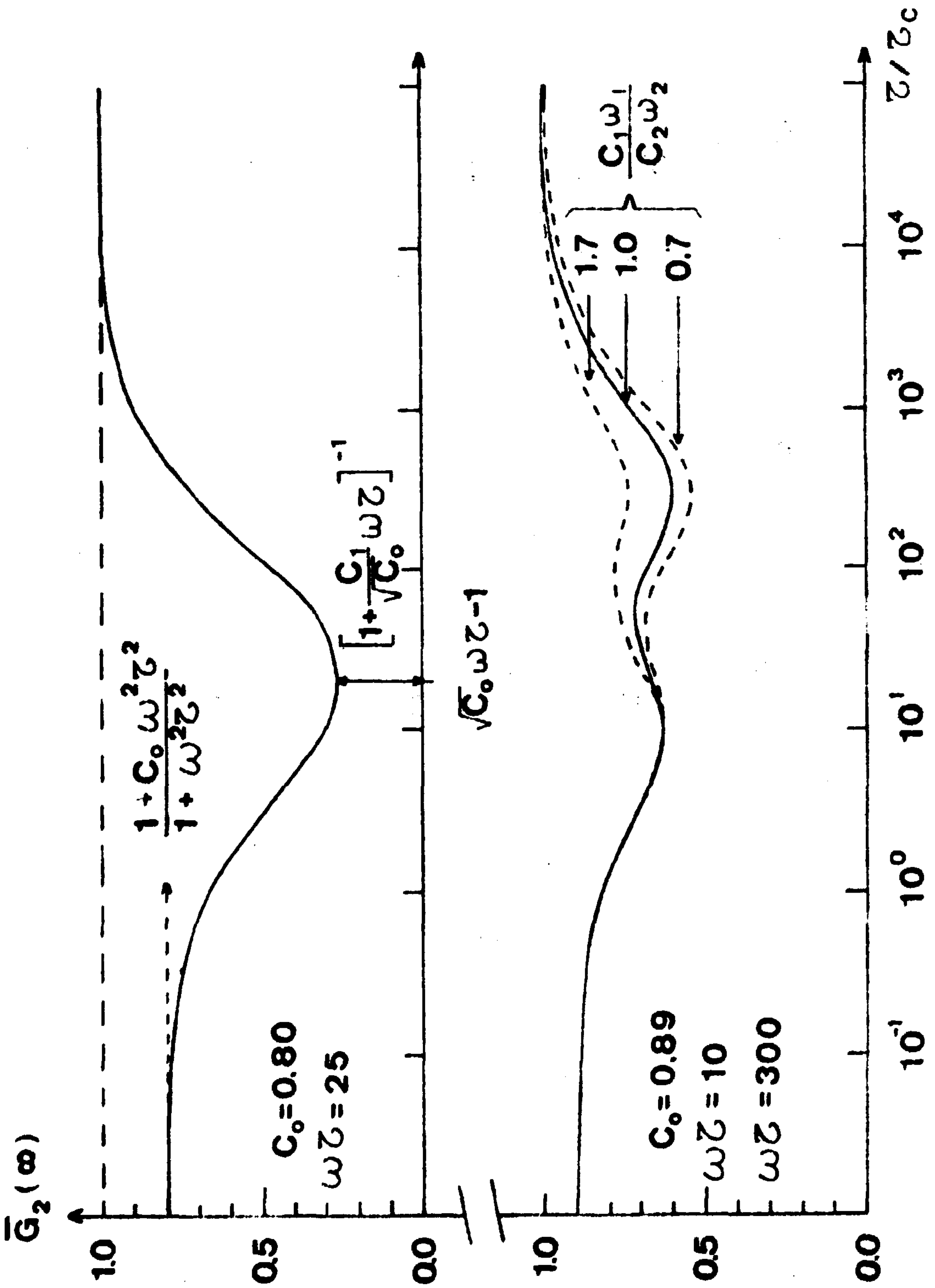
FIGURE CAPTIONS

Figure 1a (upper) - Prediction of $\overline{G_2}(\infty)$ for only one frequency with modulus different from zero.

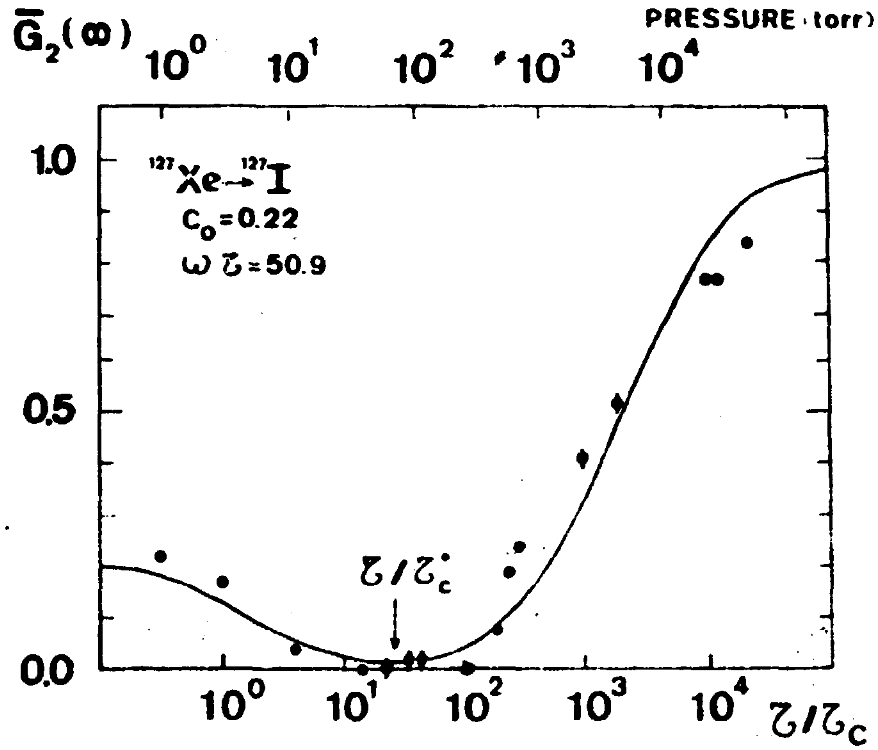
Figure 1b (lower) - The existence of minima in $\overline{G_2}(\infty)$ is a consequence of the very different values of the two assumed frequencies. One can note that when $C_1\omega_1 = C_2\omega_2$ the depth of two minima are the same.

Figure 2 - Pressure dependence of the 172-203 KeV angular correlation in ^{127}Xe. The continous line is the prediction of the Scherer-Blume theory.



$\bar{G}_2(\omega)$
1.0
0.5
0.0
1.0
0.5
0.0
$C_o = 0.80$
$\omega\tau = 25$
$C_o = 0.89$
$\omega\tau = 10$
$\omega\tau = 300$
$\frac{1 + C_o\omega^2\tau^2}{1 + \omega^2\tau^2}$
$\left[1 + \frac{C_1}{\sqrt{C_o}}\omega\tau\right]^{-1}$
$\sqrt{C_o}\,\omega\tau - 1$
1.7
1.0
0.7
$\frac{C_1\omega_1}{C_2\omega_2}$
10^{-1}
10^0
10^1
10^2
10^3
10^4
τ/τ_c

Figure 1



$\bar{G}_2(\infty)$
PRESSURE (torr)
10^0 10^1 10^2 10^3 10^4
1.0
0.5
0.0
$^{127}Xe \rightarrow {}^{127}I$
$c_0 = 0.22$
$\omega\tau = 50.9$
τ/τ_c
10^0 10^1 10^2 10^3 10^4
τ/τ_c

Figure 2