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EFFECT OF NON-CONSTANT $\Gamma_n(\varepsilon_j)$ ON NEUTRON RESONANCE BROADENING—II. HARMONIC OSCILLATOR

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Abstract—In the computation of Doppler broadening, the usual assumption used is to ignore the dependence of $\Gamma_n(j)$ on the intermediate energy ε_j of the target atoms. This assumption has been examined for ideal gas targets and it was found that the effects of the j dependence are not significant. Here we study the j dependence for a target composed of harmonic oscillators. In this paper, we compute the resonance line shape, $W(E_n)$, for harmonic oscillator targets taking into account the dependence of the neutron level width Γ_n on the intermediate state $\Gamma_n(j)$. We compare the resonance line shapes for both constant and non-constant neutron level width. Our calculations show that the difference is not significant. Therefore, the non-constancy of Γ_n seems to be absolutely not important in calculating the broadening of neutron resonances.

INTRODUCTION

The commonly used form of the resonance line shape was developed by Bethe and Placzek (1937) under the assumption that the nuclei have a Maxwellian gas distribution of velocities.

Lamb (1939) was first to discuss and to calculate the absorption line shape for an atom which is bound in a crystal lattice. The general formula is:

$$W(E_n) = |M_r|^2 |M_c|^2 \sum_{i,j} g(\varepsilon_i) \times \frac{|\langle j| e^{i\mathbf{K}.\mathbf{R}} |i\rangle|^2}{(E_n - E_0 - \varepsilon_j + \varepsilon_i)^2 + [\Gamma(j)/2]^2}. \quad (1)$$

Where M_r and M_c are the matrix elements for radiation and compound nucleus formation, respectively, and $g(\varepsilon_i)$ is the Boltzmann distribution function. ε_i and ε_j are the energies of the initial and the intermediate atomic states $|i\rangle$ and $|j\rangle$, respectively.

Equation (1) can be written in a time-dependent representation (see Van Hove, 1954; Singwi and Sjolander, 1960):

$$W(E_n) = |M_r|^2 |M_c|^2 \sum_i \sum_j g(\varepsilon_i) \frac{2}{\Gamma} \times \mathrm{Re} \int_0^{+\infty} \frac{dt}{\hbar} \exp\left[i\left(E_n - E_0 - \varepsilon_j + \varepsilon_i + i\frac{\Gamma}{2} \right) \frac{t}{\hbar} \right] \times |\langle j| e^{i\mathbf{K}.\mathbf{R}} |i\rangle|^2. \quad (2)$$

This Breit–Wigner line shape is usually calculated with the assumption of constant $\Gamma_n(j)$. Shamaoun and Summerfield (1989) have computed the effects of the ε_j dependence of the $\Gamma(j)$ on the resonance absorption cross section for an ideal gas and found that the approximation of constant $\Gamma(j)$ is valid.

NEUTRON LEVEL WIDTH $\Gamma_n(j)$ FOR HARMONIC OSCILLATOR

The equation derived by Breit and Wigner (1936) for the neutron level width as a function of the intermediate state is:

$$\Gamma_n(j) = 2\pi |M_c|^2 \sum_{1 \neq j} |\langle 1| e^{-i\mathbf{K}'.\mathbf{R}} |j\rangle|^2 \delta(E - E_1), \quad (3)$$

where $|q_1\rangle = |1\rangle$ and $|q_j\rangle = |j\rangle$ are the initial and intermediate state.

$$E = \frac{\hbar^2 K^2}{2m} + \varepsilon_i, \quad E_1 = \frac{\hbar^2 K'^2}{2m} + \varepsilon_1. \quad (4)$$

For the harmonic oscillator, the energy eigenvalues are:

$$\varepsilon_i = \hbar\omega_0 (i + \tfrac{1}{2}), \quad i = 0, 1, 2, \ldots \quad (5)$$

ω_0 is the harmonic oscillator frequency.

We can write (3) as (see Shamaoun and Summerfield, 1989):

$$\Gamma_n(j) = |M_c|^2 \sum_{\mathbf{K}'} \int_{-\infty}^{+\infty} \frac{dt}{\hbar} \cdot \exp\left[-i\left(E - \frac{\hbar^2 K'^2}{2\mu_m}\right)\frac{t}{\hbar}\right] \times \left\langle j \left| \exp\left(i\frac{t}{\hbar}H_A - i\frac{\mathbf{K}'.\mathbf{P}}{M}t\right) \right| j \right\rangle, \quad (6)$$

where H_A is the system Hamiltonian and μ_m is the reduced mass. Let us deal with the last term of equation (6) which we call d:

$$d = \left\langle j \left| \exp\left(iH_A \frac{t}{\hbar} - i\frac{\mathbf{K}'.\mathbf{p}}{M}t\right) \right| j \right\rangle. \quad (7)$$

For an isotropic harmonic potential, we get:

$$d = \langle j | \exp[i\omega_0(a^+ a + \tfrac{1}{2})t - \gamma(a - a^+)t] | j \rangle, \quad (8)$$

where a and a^+ are the lowering and the raising operators for the harmonic oscillator and

$$\gamma = \sqrt{\frac{K'^2 \hbar\omega_0}{2M}}. \quad (9)$$

We can approximate equation (8) as follows:

$$d = e^{A + Bt + Ct^2 + \cdots}. \quad (10)$$

The coefficients A, B and C are:

$$A = 0, \qquad B = i\omega_0 z, \qquad C = -\gamma^2 z,$$

where $z = j + \frac{1}{2}$.
Substituting into equation (6) we get:

$$\Gamma_n(j) = |M_c|^2 \sum_{\mathbf{K}'} \int_{-\infty}^{+\infty} \frac{dt}{\hbar} \times \exp\left\{-\gamma^2 z t^2 + i\left[\omega_0 z - \frac{1}{\hbar}\left(E - \frac{\hbar^2 K'^2}{2\mu_m}\right)\right]t\right\}. \quad (11)$$

As an approximation, we ignore terms of order t^2 in (11) (see Appendix). This gives:

$$\Gamma_n(j) = 2\pi |M_c|^2 \sum_{\mathbf{K}'} \delta\left(E - \hbar\omega_0 z - \frac{\hbar^2 K'^2}{2\mu_m}\right). \quad (12)$$

It is convenient to make the transition from discrete to continuous variables:

$$\sum_{\mathbf{K}'} \to \frac{1}{(2\pi)^3} \int d^3\mathbf{K}', \quad (13)$$

to get

$$\Gamma_n(j) = \frac{1}{\pi}|M_c|^2 \int K'^2 \delta\left(E - \hbar\omega_0 z - \frac{\hbar^2 K'^2}{2\mu_m}\right) dK'. \quad (14)$$

This integral can be done with the following result if E_n is much larger than ε_i or ε_j:

$$\Gamma_n(j) = \Gamma_n^0 \left(1 + \frac{\varepsilon_i - \varepsilon_j}{E_n}\right)^{1/2}, \quad (15)$$

where

$$\Gamma_n^0 = \frac{\sqrt{2}}{\pi} \frac{\mu_m^{3/2}}{\hbar^3} |M_c|^2 \sqrt{E_n}, \quad (16)$$

$$E_n = \frac{\hbar^2 K'^2}{2m}. \quad (17)$$

Equation (15) displays the neutron level width dependence upon ε_j. Since E_n is much greater than $(\varepsilon_i - \varepsilon_j)$ we can write:

$$\Gamma_n(j) \approx \Gamma_n^0 \left(1 + \frac{1}{2}\frac{\varepsilon_i - \varepsilon_j}{E_n}\right). \quad (18)$$

To calculate the effect of the ε_j dependence of $\Gamma(j)$ on the scattering cross section for harmonic oscillator, we need the total level width $\Gamma(j)$ which is equal to the γ-level width plus the neutron level width:

$$\Gamma(j) = \Gamma_\gamma + \Gamma_n(j). \quad (19)$$

Using equation (18), we get:

$$\Gamma(j) = \Gamma\left(1 + \frac{\Gamma_n^0}{2\Gamma}\frac{\varepsilon_i - \varepsilon_j}{E_n}\right), \quad (20)$$

where

$$\Gamma = \Gamma_\gamma + \Gamma_n^0. \quad (21)$$

Using equation (20), taking the inverse and expanding, we get:

$$\frac{1}{\Gamma(j)} = \frac{1}{\Gamma} - \frac{\Gamma_n^0}{2\Gamma^2}\frac{\varepsilon_i - \varepsilon_j}{E_n}. \quad (22)$$

Substituting equations (20) and (22) into equation (2) gives:

$$W(E_n) = |M_c|^2 |M_r|^2 \left(\frac{2}{\Gamma} + \frac{\Gamma_n^0}{\Gamma^2 E_n}\frac{\hbar^2 K^2}{2M}\right) \times \mathrm{Re} \int_0^{+\infty} \frac{dt}{\hbar} \exp\left\{\left[-\frac{\Gamma}{2} + i(E_n - E_0)\right]\frac{t}{\hbar}\right\} \times \langle e^{-iKx(\tau)} e^{iKx(0)} \rangle_T, \quad (23)$$

where

$$\langle e^{-iKx(t)}\, e^{iKx(0)}\rangle_T = \sum_i g(\varepsilon_i) \langle i|\, e^{-iKx(t)}\, e^{iKx(0)} |i\rangle, \tag{24}$$

$$\tau = \left(1 + i\frac{\Gamma_n^0}{4E_n}\right)t \tag{25}$$

and $x(\tau)$ is the Heisenberg operator.

We can express the last term of equation (23) as follows:

$$\langle e^{-iKx(\tau)}\, e^{iKx(0)}\rangle_T = \exp\left[\frac{-K^2\hbar}{2M\omega_0}\coth(\tfrac{1}{2}\hbar\omega_0\beta)\right] \times \sum_{n=-\infty}^{+\infty} \exp(in\omega_0\tau - \tfrac{1}{2}n\hbar\omega_0\beta)\, I_n(y), \tag{26}$$

where

$$y = \frac{m}{M}\frac{E_n}{\hbar\omega_0} c\, \mathrm{sech}(\tfrac{1}{2}\hbar\omega_0\beta) \tag{27}$$

and $I_n(y)$ is the modified Bessel function of the first kind.

if we note that $I_n(y) = I_{-n}(y)$ and substitute equation (26) into (23), we get:

$$W(E_n) = V\sum_0^{\infty} \exp(-\tfrac{1}{2}n\hbar\omega_0\beta)\, I_n(y) \times \int_0^{\infty} \frac{dt}{\hbar} \exp\left[-\left(\frac{\Gamma}{2} + \frac{\Gamma_n^0}{4E_n} n\hbar\omega_0\right)\frac{t}{\hbar}\right] \times \cos\left[(E_n - E_0 + n\hbar\omega_0)\frac{t}{\hbar}\right], \tag{28}$$

where

$$V = |M_c|^2 |M_r|^2 \left(\frac{2}{\Gamma} + \frac{\Gamma_n^0}{\Gamma^2}\frac{m}{M}\right) \times \exp\left[-\frac{m}{M}\frac{E_n}{\hbar\omega_0}\coth(\tfrac{1}{2}\hbar\omega_0\beta)\right]. \tag{29}$$

Then, the resonance line shape for non-constant level width is:

$$W(E_n) = V\sum_{n=0}^{\infty} \exp(-\tfrac{1}{2}n\hbar\omega_0\beta)\, I_n(y) \times \frac{\dfrac{\Gamma}{2} + \dfrac{\Gamma_n^0}{4E_n} n\hbar\omega_0}{\left(\dfrac{\Gamma}{2} + \dfrac{\Gamma_n^0}{4E_n} n\hbar\omega_0\right)^2 + (E_n - E_0 + n\hbar\omega_0)^2}. \tag{30}$$

For a constant Γ the resonance line shape $W_c(E_n)$ is:

$$W_c(E_n) = U\sum_{n=0}^{+\infty} \exp(-\tfrac{1}{2}n\hbar\omega_0\beta)\, I_n(y) \times \frac{\dfrac{\Gamma}{2}}{\left(\dfrac{\Gamma}{2}\right)^2 + (E_n - E_0 + n\hbar\omega_0)^2}, \tag{31}$$

where

$$U = |M_c|^2 |M_r|^2 \frac{2}{\Gamma} \exp\left[-\frac{m}{M}\frac{E_n}{\hbar\omega_0}\coth(\tfrac{1}{2}\hbar\omega_0\beta)\right]. \tag{32}$$

Equations (31) and (30) give the resonance line shape for the constant and non-constant Γ, respectively.

CONCLUSION AND RESULTS

We have done numerical calculations of the resonance line shapes given in equations (31) and (30) for two different isotopes with low lying resonances. The parameters for these resonances are shown in Table 1.

We have done the computations for $T = 4$, 100 and 300 K. We show the results for $T = 100$ K in Tables 2 and 3. The differences between the constant and non-constant cases are not significant. Therefore, the effect of the dependence of $\Gamma_n(j)$ on the intermediate state of the target is not significant for the harmonic oscillator as well as the ideal gas and the assumption of constant neutron level width is a valid approximation

Table 1. Parameters of some low-energy resonances

Isotope	E (eV)	Γ_γ (meV)	Γ_n (meV)	Γ_t (meV)
^{238}U	6.67	26	1.5	27.5
^{240}Pu	1.0	34	2.5	36.5

Table 2. Resonance line shape for ^{238}U

E_n (eV)	$W_c(E_n)$ $\hbar w_0 = 0.01$	$W(E_n)$ $\hbar w_0 = 0.01$	$W_c(E_n)$ $\hbar w_0 = 0.05$	$W(E_n)$ $\hbar w_0 = 0.05$
6.60	0.029664	0.029698	0.011421	0.011424
6.63	0.144527	0.144529	0.032275	0.032283
6.64	0.246001	0.245989	0.052592	0.052603
6.65	0.408724	0.408678	0.096935	0.096955
6.66	0.600036	0.599937	0.197245	0.197285
6.67	0.644537	0.645419	0.301273	0.301333
6.675	0.536817	0.536741	0.265974	0.266028
6.68	0.393611	0.393582	0.196885	0.196924
6.69	0.198897	0.198903	0.0965397	0.096559
6.70	0.111635	0.111643	0.052177	0.052188
6.72	0.047721	0.047726	0.021100	0.021104
6.74	0.026053	0.026056	0.011132	0.011134
6.76	0.016328	0.001633	0.006824	0.006825
6.80	0.008103	0.008103	0.003299	0.003300

Table 3. Resonance line shape for ^{240}Pu

E (eV)	$W_c(E_n)$ $\hbar w_0 = 0.01$	$W(E_n)$ $\hbar w_0 = 0.01$	$W_c(E_n)$ $\hbar w_0 = 0.05$	$W(E_n)$ $\hbar w_0 = 0.05$
0.92	0.009743	0.009745	0.013767	0.013769
0.94	0.016859	0.016862	0.023550	0.023554
0.95	0.023651	0.023656	0.032662	0.032668
0.96	0.035173	0.035179	0.047784	0.047791
0.97	0.055899	0.055900	0.074797	0.074809
0.98	0.092993	0.093006	0.125675	0.125695
0.99	0.146246	0.146269	0.212538	0.212571
0.995	0.168062	0.168095	0.256944	0.256984
1.00	0.173506	0.173545	0.276112	0.276155
1.005	0.157590	0.157627	0.256726	0.256765
1.01	0.128877	0.128906	0.212176	0.212209
1.02	0.075856	0.075871	0.125241	0.125260
1.03	0.045248	0.045256	0.074395	0.074406
1.04	0.028667	0.028672	0.047416	0.047423
1.05	0.019815	0.019818	0.032326	0.032331
1.10	0.005428	0.005429	0.008826	0.008828

in both cases. There is an equally small effect of non-constant $\Gamma_n(j)$ for $T = 4$ and 300 K.

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APPENDIX

We start with equation (11):

$$\Gamma_n(j) = |M_c|^2 \sum_{\mathbf{K}'} \int_{-\infty}^{+\infty} \frac{dt}{\hbar} \times \exp\left\{-\gamma^2 z t^2 + i\left[\omega_0 z - \frac{1}{\hbar}\left(E - \frac{\hbar^2 K'^2}{2\mu_m}\right)\right]t\right\}, \quad (A1)$$

which can be written in the following form:

$$\Gamma_n(j) = |M_c|^2 \sum_{\mathbf{K}'} \int_{-\infty}^{+\infty} \frac{dt}{\hbar} \times \exp(-\gamma^2 z t^2)\,[\cos(bt) + i\sin(bt)], \quad (A2)$$

where

$$b = \omega_0 z - \frac{1}{\hbar}\left(E - \frac{\hbar^2 K'^2}{2\mu_m}\right). \quad (A3)$$

The imaginary part of this function is zero. The real part is:

$$\Gamma_n(j) = |M_c|^2 \sum_{\mathbf{K}'} \frac{1}{\hbar}\sqrt{\frac{\pi}{\gamma^2 z}} \exp[-b^2/(4\gamma^2 z)]. \quad (A4)$$

To solve this equation, it is convenient to change the summation over $\mathbf{K}'$ to summation over energy and make the transition from discrete to continuous variables:

$$\Gamma_n(j) = \frac{\sqrt{\pi}}{2\pi^2\hbar}|M_c|^2 \int \frac{E_n^2}{\sqrt{\gamma^2 z}} \exp[-b^2/(4\gamma^2 z)]\,dE_n, \quad (A5)$$

Table A1

z	Equation (A6)	Equation (15)
5.5	10.904	11.109
10.5	10.911	10.923
15.5	10.725	10.738
20.5	10.546	10.555
25.5	10.368	10.375
30.5	10.191	10.194

where γ is given in equation (9). Numerical calculations of the neutron width using equations (A5) and (15) are shown in Table A1. These are very close, which justifies our approximation of neglecting terms of order t^2 in equation (11).