# THE EFFECT OF NON-CONSTANT $\Gamma_{\mathrm{n}}$ ON THE RESONANT ABSORPTION OF NEUTRONS 

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#### Abstract

A key assumption in the usual computations of Doppler broadening is to ignore the dependence of $\Gamma(j)$ on the state of the compound nucleus. This is an excellent approximation for the $\gamma$-emission contribution to $\Gamma(j)$. It is not so clear that it is as good for the neutron contribution. In this paper, we derive an expression for $\Gamma_{\mathrm{n}}(j)$ and show that the effect of the dependence of $\Gamma_{\mathrm{n}}(j)$ on the intermediate energy of the target $\varepsilon_{j}$ is not significant for an ideal gas, so that the absorption line shape is identical to the absorption line shape in which $\Gamma_{\mathrm{n}}$ is constant. Therefore, the effects of $j$ dependence $\Gamma_{\mathrm{n}}(j)$ on the absorption cross section is not significant.


## 1. INTRODUCTION

The broadening of neutron scattering and absorption resonances by thermal motion of the target atoms is referred to as "Doppler broadening". Doppler broadening is known to depend upon the state of the atom from which the scattering occurs. That is, it depends upon whether the atom is in a liquid, a solid, or a gas. This dependence is called the chemical binding effect.

The general formulation of the resonance line shape, developed by Bethe and Placzek (1937) is the psi function $\psi(\xi, x)$, calculated under the assumption that the nuclei have a Maxwellian gas distribution of velocities. This function is given by :

$$
\begin{equation*}
\psi(\xi, x)=\frac{\xi}{2 \sqrt{\pi}} \int_{-\infty}^{\infty} \mathrm{d} y \frac{\exp \left[-\frac{\xi^{2}}{4}(x-y)^{2}\right]}{1+y^{2}} \tag{1}
\end{equation*}
$$

where

$$
\begin{gather*}
\xi=\frac{\Gamma}{\Delta}  \tag{2}\\
x=\frac{2}{\Gamma}\left(E_{\mathrm{n}}-E_{0}-R\right) \tag{3}
\end{gather*}
$$

The Doppler width $\Delta$ is given by $\Delta=2(R / \beta)^{1 / 2}$ where $\beta^{-1}$ is the temperature (multiplied by Boltzmann constant $k_{\mathrm{B}}$ ) in energy units, $E_{\mathrm{n}}$ is the kinetic energy of the neutron, and $E_{0}$ is the resonance energy.

The chemical binding effect was first discussed by Lamb in (1939). He realized that the assumption of Maxwellian distribution of velocities for the absorbing nuclei is not valid if the target particles are bound in a solid. He was able to derive a formula for the absorption line shape for bound nuclei which is determined by the Debye theory of crystal lattice dynamics. The general formula is given by:

$$
\begin{equation*}
W\left(E_{\mathrm{n}}\right)=\left|M_{\mathrm{rad}}\right|^{2}\left|M_{\mathrm{comp}}\right|^{2} \sum_{i} \sum_{j} g\left(\varepsilon_{i}\right) \frac{\left.\left|\langle j| \mathrm{e}^{i \mathbf{k} \cdot \mathbf{R}_{L}}\right| i\right\rangle\left.\right|^{2}}{\left(E_{\mathrm{n}}-E_{0}-\varepsilon_{j}+\varepsilon_{i}\right)^{2}+\left(\frac{\Gamma(j)}{2}\right)^{2}}, \tag{4}
\end{equation*}
$$

where $\left|M_{\text {rad }}\right|^{2}$ and $\left|M_{\text {comp }}\right|^{2}$ are the matrix elements for radiation and compound nucleus formation, respectively, $g\left(\varepsilon_{i}\right)$ is the probability of finding the target in the state $i .|i\rangle$ and $|j\rangle$ are the initial and the intermediate state
of the target, respectively, and the $\varepsilon s$ are the target energy. It was Lamb's work which led Mössbauer (1958) to his results for resonant absorption of $\gamma$-rays.

A different form is obtained by transforming equation (4) into a time dependent representation (Singwi and Sjolander, 1960 ; Van Hove, 1954)

$$
\begin{gather*}
\left.W\left(E_{\mathrm{n}}\right)=\left|M_{\mathrm{rad}}\right|^{2}\left|M_{\text {comp }}\right|^{2} \sum_{i} \sum_{j} g\left(\varepsilon_{i}\right)\left|\langle j| \mathrm{e}^{i \mathbf{K} \cdot \mathbf{R}_{L}}\right| i\right\rangle\left.\right|^{2} \frac{2}{\Gamma} \operatorname{Re} \int_{0}^{\infty} \frac{\mathrm{d} t}{\hbar} \mathrm{e}^{i\left(E_{\mathrm{n}}-E_{0}-\varepsilon_{j}+\varepsilon_{i}+(i \Gamma / 2)\right) t / \hbar},  \tag{5}\\
\left.W\left(E_{\mathrm{n}}\right)=\left.\left|M_{\mathrm{rad}}\right|^{2}\left|M_{\text {comp }}\right|^{2} \frac{2}{\Gamma} \operatorname{Re} \int_{0}^{\infty} \frac{\mathrm{d} t}{\hbar}\left\{\sum_{i} \sum_{j} g\left(\varepsilon_{i}\right)\left|\langle j| \mathrm{e}^{i \mathbf{K} \cdot \mathbf{R}_{L}}\right| i\right\rangle\right|^{2} \mathrm{e}^{i\left(\varepsilon_{i}-\varepsilon_{j}\right) t / \hbar}\right\} \mathrm{e}^{i\left(E_{\mathrm{n}}-E_{0}+(\Gamma / 2)\right) / \hbar} \tag{6}
\end{gather*}
$$

writing

$$
\begin{gather*}
\left.\left|\langle j| \mathrm{e}^{i \mathbf{K} \cdot \mathbf{R}_{L}}\right| i\right\rangle\left.\right|^{2}=\langle i| \mathrm{e}^{-i \mathbf{K} \cdot \mathbf{R}_{L}}|j\rangle\langle j| \mathrm{e}^{i \mathbf{K} \cdot \mathbf{R}_{L}}|i\rangle  \tag{7}\\
\sum_{j}|\mathrm{j}\rangle\langle j|=I \tag{8}
\end{gather*}
$$

and using

$$
\begin{align*}
\mathrm{e}^{i \varepsilon_{t} / / \hbar}|i\rangle & =\mathrm{e}^{i H_{\mathrm{A}} / / \hbar}|i\rangle  \tag{9}\\
\mathrm{e}^{-i \varepsilon_{i} / / / \hbar}|j\rangle & =\mathrm{e}^{-i H_{\mathrm{A}} / / \hbar}|j\rangle \tag{10}
\end{align*}
$$

equation (6) becomes :

$$
\begin{equation*}
W\left(E_{\mathrm{n}}\right)=\left|M_{\mathrm{rad}}\right|^{2}\left|M_{\mathrm{comp}}\right|^{2} \frac{2}{\Gamma} \operatorname{Re} \int_{0}^{\infty} \frac{\mathrm{d} t}{\hbar} \mathrm{e}^{-(\Gamma / 2)(t / /)} \mathrm{e}^{i\left(E_{\mathrm{n}}-E_{0} t t / \hbar\right.}\left\langle\mathrm{e}^{-\mathbf{K} \cdot \mathbf{R}_{L}(t)} \mathrm{e}^{i \mathbf{K} \cdot \mathbf{R}_{L}}\right\rangle_{\mathrm{T}} \tag{11}
\end{equation*}
$$

where $\mathbf{R}_{L}(t)$ is the Heisenberg operator for the position of the $L$ th nucleus at time $t$ :

$$
\begin{equation*}
\mathbf{R}_{L}(t)=\mathrm{e}^{i H(t / \hbar)} \mathbf{R}_{L}(0) \mathrm{e}^{-i H(/ / \hbar)} \tag{12}
\end{equation*}
$$

the notation $\langle\ldots\rangle_{\mathrm{T}}$ in the above equation implies that a thermal average is to be taken.
By definition:

$$
\begin{equation*}
\left\langle\mathrm{e}^{-i \mathbf{K} \cdot \mathbf{R}_{L}(t)} \mathrm{e}^{i \mathbf{K} \cdot \mathbf{R}_{L}}\right\rangle_{\mathrm{T}}=\sum_{i} g\left(\varepsilon_{i}\right)\langle i| \mathrm{e}^{-i \mathbf{K} \cdot \mathbf{R}_{L}(t)} \mathrm{e}^{i \mathbf{K} \cdot \mathbf{R}_{L}}|i\rangle \tag{13}
\end{equation*}
$$

and the distribution function is given by :

$$
\begin{equation*}
g\left(\varepsilon_{i}\right)=Z^{-1} \mathrm{e}^{-\beta \varepsilon_{i}}, \quad Z=\sum_{i} \mathrm{e}^{-\beta \varepsilon_{i}} \tag{14}
\end{equation*}
$$

It has been shown by Van Hove (1954) that for a perfect gas, the quantum mechanical form of the matrix element is :

$$
\begin{equation*}
\left\langle\mathrm{e}^{-i \mathbf{K} \cdot \mathbf{R}_{L}(t)} \mathrm{e}^{i \mathbf{K} \cdot \mathbf{R}_{L}}\right\rangle_{\mathrm{T}}=\mathrm{e}^{-i\left(\hbar \hbar K^{2} / 2 M\right)-\left(t^{2} K^{2} / 2 M \beta\right)} \tag{15}
\end{equation*}
$$

If we substitute (15) in (11), we get :

$$
\begin{equation*}
W\left(E_{\mathrm{n}}\right)=\left|M_{\mathrm{rad}}\right|^{2}\left|M_{\mathrm{comp}}\right|^{2} \frac{2}{\Gamma} \operatorname{Re} \int_{0} \frac{\mathrm{~d} t}{\hbar} G_{0}(t) \mathrm{e}^{A_{0}(t / \mathrm{h})} \mathrm{e}^{B_{0} t^{2}}, \tag{16}
\end{equation*}
$$

where

$$
\begin{gather*}
A_{0}=i\left(E_{\mathrm{n}}-E_{0}-R+\frac{i \Gamma}{2}\right), \quad R=\frac{\hbar^{2} K^{2}}{2 M}  \tag{17}\\
B_{0}=-\frac{R}{\beta}  \tag{18}\\
G_{0}(t)=1 \tag{19}
\end{gather*}
$$

Let us write equation (16) in terms of the psi-function:

$$
\begin{gather*}
\left.W\left(E_{\mathrm{n}}\right)=\left|M_{\mathrm{rad}}\right|^{2}\left|M_{\mathrm{comp}}\right|^{2} \frac{4}{\Gamma^{2}} \int_{0}^{\infty} \mathrm{d} y \cos y x \mathrm{e}^{-y-y^{2}} \right\rvert\, \xi^{2}  \tag{20}\\
W\left(E_{\mathrm{n}}\right)=\left|M_{\mathrm{rad}}\right|^{2}\left|M_{\mathrm{comp}}\right|^{2} \frac{4}{\Gamma^{2}} \Psi(x, \xi) \tag{21}
\end{gather*}
$$

where $\psi(x, \xi) \dagger, x$ and $\xi$ are defined by equations (1-3) and the dimensionless variable can be introduced by:

$$
y=\frac{\Gamma}{2} \frac{t}{\hbar}
$$

## 2. THEORY OF THE CHEMICAL BINDING EFFECT ON RESONANT ABSORPTION OF NEUTRONS

We shall begin by examining the underlying approximations made in obtaining the Breit-Wigner cross sections and the connection of these expressions to the states of the target atoms. We can write both the absorption and scattering cross sections in terms of the $T$-matrix (Rodberg and Thaler, 1967):

$$
\begin{equation*}
T=V+V\left(E-H_{0}-V+i \varepsilon\right)^{-1} V \tag{22}
\end{equation*}
$$

where $V$ is the operator for the interaction and $H_{0}$ is the operator which describes the relative motion and internal properties of the colliding particles.

The cross sections are, of course, proportional to the matrix elements of $T$. The Breit-Wigner cross sections are obtained by assuming that the off-diagonal elements of $\left(E-H_{0}-V+i \varepsilon\right)$ are zero and expanding as follows :

$$
\begin{equation*}
\left\{\langle j| \frac{1}{E-H_{0}-\lambda H^{\prime}+i \varepsilon}|j\rangle\right\}^{-1}=E-E_{j}-\langle j| V|j\rangle+\frac{(\langle j| V|j\rangle)^{2}}{E-E_{j}+i \varepsilon}-\langle j| V(E-H+i \varepsilon)^{-1} V|j\rangle+\ldots \tag{23}
\end{equation*}
$$

after some manipulation, this permits us to write the matrix elements of $T$ as:

$$
\begin{equation*}
\langle f| T|i\rangle=\langle f| V|j\rangle+\sum_{j} \frac{\langle f| V|j\rangle\langle j| V|i\rangle}{E-E_{0}+\frac{i \Gamma(j)}{2}}+\cdots \tag{24}
\end{equation*}
$$

where

$$
\begin{equation*}
E_{0}=E_{j}+\langle j| V|j\rangle+P \sum_{1 \neq j} \frac{\langle j| V|l\rangle\langle l| V|j\rangle}{E-E_{l}}+\cdots \tag{25}
\end{equation*}
$$

$P$ indicates the principal value. $\Gamma(j)$ is :

$$
\begin{equation*}
\Gamma(j)=2 \pi \sum_{\neq j}\langle j| V|l\rangle\langle l| V|j\rangle \delta\left(E-E_{l}\right)+\cdots \tag{26}
\end{equation*}
$$

Every one takes the total $\Gamma(j)$ and partial $\Gamma_{\mathrm{n}}(j)$ level width to be energy independent. We will write an expression for the chemical binding effects on $\Gamma(j)$. This is what Lamb (1939) calls $\Gamma\left(n_{s}\right)$ :

$$
\begin{equation*}
\Gamma\left(n_{\mathrm{s}}\right)=\Gamma_{\gamma}+\Gamma_{\mathrm{n}}\left(n_{\mathrm{s}}\right) \tag{27}
\end{equation*}
$$

remember that $V$ is the interaction potential binding the scatterer. However, if a photon is produced in the intermediate state, we must account for the interaction potential between the electromagnetic field and the produced photon (Davydov, 1966) :

$$
\begin{equation*}
V=V_{\text {neutron }}+\sum_{\mu} \frac{q}{m c} A\left(r_{\mu}\right) \cdot P_{\mu} \tag{28}
\end{equation*}
$$

$\dagger$ To obtain equation (21), it is necessary to use the integral representation :

$$
\frac{1}{1+x^{2}}=\int_{0}^{\infty} \mathrm{e}^{-s} \cos (s x) \mathrm{d} s
$$

the second term is the operator for the interaction of a spinless particle of mass $(m)$ and charge $(q)$ with an electromagnetic field, where $\mu$ indicates the number of charge particles in the nucleus.

The electromagnetic field, which is described by the vector potential $A$, has the form:

$$
\begin{equation*}
A(\mathbf{r})=(2 \pi h c)^{1 / 2} \sum_{\mathbf{Q} \cdot \alpha} \frac{\mathbf{e}_{\mathbf{Q} \alpha}}{\sqrt{Q}}\left\{a_{\mathbf{Q}_{\alpha}} \mathrm{e}^{i \mathbf{Q} \cdot \mathbf{r}}+a_{\mathbf{Q} x}^{+} \mathrm{e}^{i \mathbf{Q} \cdot \mathbf{r}}\right\} \tag{29}
\end{equation*}
$$

where $\mathbf{e}_{\mathbf{Q} \alpha}$ is the polarization vector; $\mathbf{Q}$ is the wave vector of the photon and $a_{\mathbf{Q}_{\alpha}}$ and $a_{\mathbf{Q}_{\alpha}}^{+}$are the operators for the creation and annihilation of quanta of electromagnetic radiation, respectively.

In order to have just $\Gamma_{n}$, we can ignore the electromagnetic term and then have pure nuclear potential :

$$
\begin{equation*}
V(r)=V_{\text {neutron }}=\sum_{v} V\left(r_{v}-r_{\mathrm{n}}\right), \quad v=1,2, \ldots, A \tag{30}
\end{equation*}
$$

where $v$ is summed over the nucleons in the nucleus.
Define the initial and final states of the system as:

$$
\begin{align*}
|i\rangle & =\Phi_{\mathrm{i}}\left(\mathbf{r}_{1}, \mathbf{r}_{2}, \ldots, \mathbf{r}_{\mathrm{A}}\right) \mathrm{e}^{i \mathbf{K} \cdot \mathbf{r}_{\mathrm{n}}}  \tag{31}\\
|f\rangle & =\Phi_{\mathrm{f}}\left(\mathbf{r}_{1}, \mathbf{r}_{2}, \ldots, \mathbf{r}_{\mathrm{A}}\right) \mathrm{e}^{i \mathbf{K}^{\prime} \cdot \mathbf{r}_{\mathrm{n}}} \tag{32}
\end{align*}
$$

where $\Phi_{\mathrm{i}}$ and $\Phi_{\mathrm{f}}$ are the initial and the final states of the scattering atom and $\mathrm{e}^{i \mathbf{K} \cdot \mathrm{r}_{\mathrm{n}}}$ and $\mathrm{e}^{i \mathbf{K} \cdot \mathbf{r}_{\mathrm{n}}}$ are the plane wave representation of the initial and final neutron state.

The intermediate state can be represented by:

$$
\begin{equation*}
|j\rangle=\Psi^{*}(\mathbf{r}) \Phi_{j}(\mathbf{R}) \tag{33}
\end{equation*}
$$

where $\Psi^{*}(\mathbf{r})$ is the excited state of the compound nucleus as function of relative coordinate $\mathbf{r}$ and $\Phi(\mathbf{R})$ is motion of the nuclei state as a function of center of mass coordinate.

$$
\begin{equation*}
R=\left(A r_{v}+r_{\mathrm{n}}\right) /(A+1) \tag{34}
\end{equation*}
$$

Then the matrix element of the potential can be written as:

$$
\begin{equation*}
V_{j 1}=\langle 1| V|j\rangle=\int d^{3} r_{\mathrm{n}} \int d^{3} r_{1}, \ldots, d^{3} r_{\mathrm{A}} \mathrm{e}^{-i \mathbf{K}^{\prime} \cdot \mathbf{r}_{\mathrm{n}}} \Phi_{1}^{*}\left(\mathbf{r}_{1}, \mathbf{r}_{2}, \ldots, \mathbf{r}_{\mathrm{A}}\right) V(\mathbf{r}) \Psi^{*}(\mathbf{r}) \Phi_{j}(\mathbf{R}) \tag{35}
\end{equation*}
$$

to reduce the complexity of this equation, we suppress the dependence of the matrix element to one variable. Also we approximate $\Phi_{j}(\mathbf{R})$ for a heavy nucleus, as:

$$
\begin{equation*}
\Phi_{j}(\mathbf{R})=\Phi_{j}\left(\frac{\left.A \mathbf{r}_{\mu}+\mathbf{r}_{\mathbf{n}}\right)}{A+1}\right)=\Phi_{j}\left(\mathbf{r}_{\mu}-\frac{\mathbf{r}}{A+1}\right) \approx \Phi_{j}\left(\mathbf{r}_{\mu}\right) \tag{36}
\end{equation*}
$$

if we replace $\mathbf{r}_{\mathrm{n}}=\mathbf{r}_{\mu}-\mathbf{r}$, equation (35) becomes:

$$
\begin{equation*}
V_{j 1}=\int d^{3} r_{\mu} \mathrm{e}^{-i \mathbf{K}^{\prime} \cdot \mathbf{r}_{\mu}} \Phi_{1}^{*}\left(\mathbf{r}_{\mu}\right) \Phi_{j}\left(\mathbf{r}_{\mu}\right) \int d^{3} r V(\mathbf{r}) \mathrm{e}^{i \mathbf{K}^{\prime} \cdot \mathbf{r}} \Psi^{*}(\mathbf{r}) \tag{37}
\end{equation*}
$$

substituting this into equation (26) we get:

$$
\begin{equation*}
\Gamma_{\mathrm{n}}(j)=2 \pi \sum_{\mathbf{1} \neq j}\left|\int d^{3} r \mathrm{e}^{i \mathbf{K}^{\prime} \cdot \mathbf{r}} V(\mathbf{r}) \Psi^{*}(\mathbf{r})\right|^{2}(x)\left|\int d^{3} r_{\mu} \Phi_{1}^{*}\left(\mathbf{r}_{\mu}\right) \mathrm{e}^{-i \mathbf{K}^{\prime} \cdot \mathbf{r}_{\mu}} \Phi_{j}\left(\mathbf{r}_{\mu}\right)\right|^{2} \delta\left(E-E_{1}\right) \tag{38}
\end{equation*}
$$

or

$$
\begin{equation*}
\left.\Gamma_{\mathrm{n}}(j)=2 \pi\left|M_{\text {comp }}\right|^{2} \sum_{1 \neq j}\left|\left\langle q_{1}\right| \mathrm{e}^{-\mathbf{K}^{\prime} \cdot \mathrm{r}_{\mathrm{u}}}\right| q_{j}\right\rangle\left.\right|^{2} \delta\left(E-E_{1}\right) \tag{39}
\end{equation*}
$$

where

$$
\begin{equation*}
\left|q_{j}\right\rangle=\Phi_{j}\left(\mathbf{r}_{\mu}\right) \quad \text { and } \quad\left|q_{1}\right\rangle=\Phi_{1}\left(\mathbf{r}_{\mu}\right) \tag{40}
\end{equation*}
$$

$$
\begin{align*}
E_{l} & =\frac{h^{2} K^{\prime 2}}{2 m}+\varepsilon_{l}  \tag{41}\\
E & =\frac{h^{2} K^{2}}{2 m}+\varepsilon_{i} \tag{42}
\end{align*}
$$

The matrix element :

$$
\begin{equation*}
\left|M_{\text {comp }}\right|^{2}=\left|\int \mathrm{d} r^{3} \mathrm{e}^{i \mathbf{K}^{\prime} \cdot \mathbf{r}} V(\mathbf{r}) \Psi^{*}(\mathbf{r})\right|^{2} \tag{43}
\end{equation*}
$$

is purely nuclear so that the range of interaction $\ll 1 / \mathbf{K}^{\prime} . \Psi^{*}(r)$ is the compound state. This factor does not depend upon chemical binding and is independent of $K^{\prime}$. For an ideal gas :

$$
\begin{equation*}
\varepsilon_{i}=\frac{h^{2} \mathbf{q}_{i}^{2}}{2 M}, \quad \varepsilon_{l}=\frac{h^{2} \mathbf{q}_{l}^{2}}{2 M} \tag{44}
\end{equation*}
$$

$\mathbf{q}_{j}$ and $\mathbf{q}_{l}$ are defined by:

$$
\begin{gather*}
\left|q_{j}\right\rangle=\mathrm{e}^{i \mathbf{q}_{j} \cdot \mathbf{r}_{\mu}}, \quad\left|q_{l}\right\rangle=\mathrm{e}^{i \mathbf{q}_{i} \cdot \mathbf{r}_{\mu}},  \tag{45}\\
\left.\left|\left\langle q_{l}\right| \mathrm{e}^{-i \mathbf{K}^{\prime} \cdot \mathbf{r}_{\mu}}\right| q_{j}\right\rangle\left.\right|^{2}=\delta\left(\mathbf{q}_{l}+\mathbf{K}^{\prime}-\mathbf{q}_{j}\right),  \tag{46}\\
\therefore \Gamma_{\mathrm{n}}(j)=2 \pi\left|M_{\text {comp }}\right|^{2} \sum_{1 \neq j} \delta\left(\mathbf{q}_{l}+\mathbf{K}^{\prime}-\mathbf{q}_{j}\right) \cdot \delta\left(E-\frac{\hbar^{2} K^{\prime 2}}{2 m}-\varepsilon_{l}\right),  \tag{47}\\
\delta\left(\mathbf{q}_{l}+\mathbf{K}^{\prime}-\mathbf{q}_{j}\right)=1, \quad \mathbf{q}_{l}=\mathbf{q}_{j}-\mathbf{K}^{\prime},  \tag{48}\\
\Gamma_{\mathrm{n}}(j)=2 \pi\left|M_{\text {comp }}\right|^{2} \sum_{K^{\prime}} \delta\left(\frac{\hbar^{2} q_{i}^{2}}{2 M}+\frac{\hbar^{2} K^{2}}{2 m}-\frac{\hbar^{2} K^{\prime 2}}{2 m}-\frac{\hbar^{2}}{2 M}\left(\mathbf{q}_{j}-\mathbf{K}^{\prime}\right)^{2}\right) . \tag{49}
\end{gather*}
$$

In order to solve this equation, it is convenient to make transition from the discrete variable to continuous case.

$$
\begin{equation*}
\sum_{K^{\prime}} \rightarrow(2 \pi)^{-3} \int d^{3} K^{\prime} \tag{50}
\end{equation*}
$$

then equation (49) becomes:

$$
\begin{equation*}
\Gamma_{\mathrm{n}}(j)=(2 \pi)^{-2}\left|M_{\mathrm{comp}}\right|^{2} \int d^{3} K^{\prime} \delta\left(\frac{\hbar^{2} q_{i}^{2}}{2 M}+\frac{\hbar^{2} K^{2}}{2 m}-\frac{\hbar^{2} K^{\prime 2}}{2 \mu_{\mathrm{m}}}-\frac{\hbar^{2} q_{j}^{2}}{2 M}+\frac{\hbar^{2}}{M} \mathbf{q}_{j} \mathbf{K}^{\prime}\right) \tag{51}
\end{equation*}
$$

where $\mu_{\mathrm{m}}$ is the neutron-nucleus reduced mass; changing variables:

$$
\begin{gather*}
\mathbf{Q}=\mathbf{K}^{\prime}+\alpha, \quad \alpha=-\frac{\mu_{\mathrm{m}}}{M} \mathbf{q}_{j}  \tag{52}\\
\Gamma_{\mathrm{n}}(j)=2(2 \pi)^{-1}\left|M_{\mathrm{comp}}\right|^{2} \int Q^{2} \mathrm{~d} Q \delta\left(\frac{\hbar^{2} q_{i}^{2}}{2 M}+\frac{\hbar^{2} K^{2}}{2 m}-\frac{\hbar^{2} q_{j}^{2}}{2 M}+\frac{\hbar^{2} \mu_{\mathrm{m}}}{2 M^{2}} q_{j}^{2}-\frac{\hbar^{2} Q^{2}}{2 \mu_{\mathrm{m}}}\right) \tag{53}
\end{gather*}
$$

Again we define a new variable:

$$
\begin{gather*}
S=\frac{\hbar^{2}}{2 \mu_{\mathrm{m}}} Q^{2}, \quad \mathrm{~d} S=\frac{\hbar^{2}}{\mu_{\mathrm{m}}} Q \mathrm{~d} Q  \tag{54}\\
\Gamma_{\mathrm{n}}(j)=\left(\frac{2 \mu_{\mathrm{m}}}{h^{2}}\right)^{3 / 2} \frac{\left|M_{\mathrm{comp}}\right|^{2}}{2 \pi} \int S^{1 / 2} \mathrm{~d} S \delta\left(\frac{\hbar^{2} q_{i}^{2}}{2 M}+\frac{\hbar^{2} K^{2}}{2 m}-\frac{\hbar^{2} q_{j}^{2}}{2}\left(\frac{1}{m+M}\right)-S\right) \tag{55}
\end{gather*}
$$

perform the integration and get:

$$
\begin{equation*}
\Gamma_{\mathrm{n}}(j)=\Gamma_{\mathrm{n}}^{0}\left(1+\frac{\varepsilon_{i}}{E_{\mathrm{n}}}-\frac{M}{m+M} \frac{\varepsilon_{j}}{E_{\mathrm{n}}}\right)^{1 / 2}, \quad \Gamma_{\mathrm{n}}^{0} \equiv\left(\frac{2 \mu_{\mathrm{m}}}{\hbar^{2}}\right)^{3 / 2} \frac{\left|M_{\mathrm{comp}}\right|^{2}}{2 \pi} \sqrt{E_{\mathrm{n}}} \tag{56}
\end{equation*}
$$

This equation indicates that $\Gamma_{\mathrm{n}}$ is $\varepsilon_{j}$ dependent. Therefore there must be an effect on $\Gamma_{\mathrm{n}}$. However, if the neutron energy is large in comparison with the total level width, then it is a good approximation to neglect this energy dependence.

We approximate the above equation for heavy nuclei as:

$$
\begin{equation*}
\Gamma_{\mathrm{n}}(j)=\Gamma_{\mathrm{n}}^{0}\left(1+\frac{1}{2} \frac{\varepsilon_{i}-\varepsilon_{j}}{E_{\mathrm{n}}}\right) \tag{57}
\end{equation*}
$$

Let us find out the effect of the chemical binding at zero temperature:

$$
\begin{equation*}
W\left(E_{\mathrm{n}}\right)=\left|\mathrm{M}_{\mathrm{rad}}\right|^{2}\left|M_{\mathrm{comp}}\right|^{2} \sum_{i, j} g\left(\varepsilon_{i}\right) \frac{\delta\left(\mathbf{q}_{i}+K-\mathbf{q}_{j}\right)}{\left(E_{\mathrm{n}}-E_{0}-\varepsilon_{j}+\varepsilon_{i}\right)+\left(\frac{\Gamma(j)}{2}\right)} \tag{58}
\end{equation*}
$$

at $T=0, \varepsilon_{i}=0$, and

$$
\begin{equation*}
\mathbf{q}_{j}=\mathbf{q}_{i}+\mathbf{K}=\mathbf{K} \quad \text { then } \quad \varepsilon_{j} / E_{\mathrm{n}}=m / M \quad \text { and } \quad \Gamma=\Gamma_{\mathrm{n}}^{0} \sqrt{\frac{M}{m+M}} \tag{59}
\end{equation*}
$$

Therefore there is no effect on $\Gamma_{\mathrm{n}}$ at $T=0$

## 3. THE CORRECTED RESONANCE LINE SHAPE EQUATION

To compute the effect of the $\varepsilon_{j}$ dependence of $\Gamma(j)$ on the absorption cross section for an ideal gas, we start from equation (5) and write :

$$
\begin{equation*}
W\left(E_{\mathrm{n}}\right)=\left|M_{\mathrm{rad}}\right|^{2}\left|M_{\mathrm{comp}}\right|^{2} \sum_{i} g\left(\varepsilon_{i}\right) \sum_{j} \frac{2}{\Gamma(j)} \operatorname{Re} \int_{0}^{\infty} \frac{\mathrm{d} t}{\hbar} \mathrm{e}^{i\left(E_{\mathrm{n}}-E_{0}-\varepsilon_{j}+\varepsilon_{i}+(i \Gamma(j) / 2)\right) t / h} \delta\left(\mathbf{q}_{i}+\mathrm{K}-\mathbf{q}_{j}\right) \tag{60}
\end{equation*}
$$

We use an ideal gas for simplicity and to give us an order of magnitude estimate of the size of the correction from nonconstant $\Gamma_{\mathrm{n}}$.

Now we use equation (57) and use the expansion:

$$
\begin{equation*}
\frac{2}{\Gamma(j)}=\frac{2}{\Gamma_{\gamma}+\Gamma_{\mathrm{n}}^{0}}-\frac{\Gamma_{\mathrm{n}}^{0}}{\left(\Gamma_{\gamma}+\Gamma_{\mathrm{n}}^{0}\right)^{2}}\left(\frac{\varepsilon_{i}-\varepsilon_{j}}{E_{\mathrm{n}}}\right) \tag{61}
\end{equation*}
$$

and perform the summation over $i$. Then equation (60) becomes:

$$
\begin{equation*}
W\left(E_{\mathrm{n}}\right)=C \frac{2}{\Gamma} \operatorname{Re} \int_{0}^{\infty} \frac{\mathrm{d} t}{\hbar} G(t) \mathrm{e}^{A / / \hbar+B t^{2}}, \quad \Gamma=\Gamma_{\gamma}+\Gamma_{\mathrm{n}}^{0} \tag{62}
\end{equation*}
$$

where:

$$
\begin{gather*}
A=-\frac{\Gamma}{2}+i\left(E_{\mathrm{n}}-E_{0}-R\right)+\Gamma_{\mathrm{n}}^{0} \frac{m}{4 M},  \tag{63}\\
B=\frac{R}{\beta}\left\{\left(\frac{\Gamma_{\mathrm{n}}^{0}}{4 E_{\mathrm{n}}}\right)^{2}-1-i \frac{\Gamma_{\mathrm{n}}^{0}}{2 E_{\mathrm{n}}}\right\},  \tag{64}\\
G(t)=1+\left(\frac{\Gamma_{\mathrm{n}}^{0}}{\Gamma} \frac{m}{2 M}\right)\left(1+\frac{\Gamma_{\mathrm{n}}^{0}}{2 \beta \hbar E_{\mathrm{n}}} t-i \frac{2 t}{\beta \hbar}\right), \tag{65}
\end{gather*}
$$

we can see that the corrections to $B_{0}$ are of order $\Gamma_{\mathrm{n}}^{0} / E_{\mathrm{n}}$ and the corrections to $A_{0}$ and $G_{0}(t)$ are of order $m / M$. Thus we do not expect the contributions from these corrections to be significant.

Let us write equation (62) in terms of a modified psi-function $\Psi(X, \eta)$ :

$$
\begin{equation*}
\Psi(X, \eta)=\int_{0}^{\infty} \mathrm{d} Y[\gamma \cos X Y+Y(\tau \cos X Y+v \sin X Y)] \mathrm{e}^{(y-2) \gamma-\left(\gamma^{2} / \eta^{2}\right)} \tag{66}
\end{equation*}
$$

where

$$
\begin{aligned}
& X Y=x y-w y^{2} / \xi^{2}, \\
& Y=\Gamma t / 2 \hbar \\
& \gamma=1+(m / M)\left(\Gamma_{\mathrm{n}}^{0} / 2 \Gamma\right) \\
& \tau=\left(m / \beta M E_{\mathrm{n}}\right)\left(\Gamma_{\mathrm{n}}^{02} / 2 \Gamma^{2}\right), \\
& \eta^{2}=\xi^{2} /\left[1-(w / 2)^{2}\right] \\
& w=\Gamma_{\mathrm{n}}^{0} / 2 E_{\mathrm{n}}, \quad v=4 E_{\mathrm{n}} \tau / \Gamma_{\mathrm{n}}^{0}
\end{aligned}
$$

the new Doppler width is:

$$
\begin{equation*}
\Delta_{\mathrm{D}}=\Delta\left[1-\left(\frac{w}{2}\right)^{2}\right] \tag{67}
\end{equation*}
$$

## 4. RESULT AND DISCUSSION

Now we present the results of the resonance line shape of the neutron absorption. Table 1 gives the psifunctions which were expressed by equations (20) and (64) for the 6.67 eV resonance at two different temperatures : 4 and 1000 K . The difference in the results from equations (20) and (64) for either $T=4$ or $T=1000 \mathrm{~K}$ increases as we reach the resonance energy (order of $10^{-4}$ ). The differences are not significant, so that Fig. 1 shows that the resonance line shapes given by equations (20) and (64) are identical for $T=4 \mathrm{~K}$ and Fig. 2 shows also the same for $T=1000 \mathrm{~K}$. Both figures are centered at 6.67 eV plus the nucleus recoil

Table 1. The psi-function at 6.67 eV resonance of ${ }^{238} \mathrm{U}$

|  | $T=4 \mathrm{~K}$ |  | $T=1000 \mathrm{~K}$ |  |
| :--- | :--- | :--- | :--- | :--- |
| $E(\mathrm{eV})$ | $\Psi(x, \xi)$ |  | $\Psi(X, \eta)$ |  |
| 6.50 | $0.48376 \mathrm{E}-2$ | $0.48376 \mathrm{E}-2$ | $0.11379 \mathrm{E}-1$ | $0.11383 \mathrm{E}-1$ |
| 6.60 | $0.19518 \mathrm{E}-1$ | $0.19518 \mathrm{E}-1$ | $0.93211 \mathrm{E}-1$ | $0.93223 \mathrm{E}-1$ |
| 6.66 | 0.11946 | 0.11947 | 0.18780 | 0.18787 |
| 6.67 | 0.20292 | 0.20295 | 0.19890 | 0.19896 |
| 6.68 | 0.38708 | 0.38717 | 0.20701 | 0.20707 |
| 6.69 | 0.73460 | 0.73493 | 0.21170 | 0.21177 |
| 6.70 | 0.90747 | 0.90799 | 0.21273 | 0.21281 |
| 6.71 | 0.59219 | 0.59244 | 0.21006 | 0.21014 |
| 6.72 | 0.30103 | 0.30112 | 0.20386 | 0.20394 |
| 6.73 | 0.16452 | 0.16453 | 0.19446 | 0.19454 |
| 6.74 | 0.10081 | 0.10082 | 0.18236 | 0.18245 |
| 6.75 | $0.67461 \mathrm{E}-1$ | $0.67464 \mathrm{E}-1$ | 0.16818 | 0.16826 |
| 6.80 | $0.18141 \mathrm{E}-1$ | $0.18141 \mathrm{E}-1$ | $0.88522 \mathrm{E}-1$ | $0.88563 \mathrm{E}-1$ |
| 6.90 | $0.46622 \mathrm{E}-2$ | $0.46622 \mathrm{E}-2$ | $0.11381 \mathrm{E}-1$ | $0.11380 \mathrm{E}-1$ |



Fig. 1. The 6.67 eV resonance line shape of ${ }^{238} \mathrm{U}$ at $T=4 \mathrm{~K}$.


Fig. 2. The 6.67 eV resonance line shape of ${ }^{238} \mathrm{U}$ at $T=$ 1000 K .
energy. Therefore our results indicate that the nonconstancy of $\Gamma_{n}$ is not an important effect in calculating the broadening of the resonance cross sections.
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