NEUTRON TRANSFER KERNELS IN THE RESONANCE DOMAIN IN THE HARMONIC CRYSTAL MODEL

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ABSTRACT

To describe neutron scattering in the resonance domain of the nuclear fuel isotopes, the static model is widely in use in nuclear data processing codes. With this model the influence of chemical binding on the transfer cross section is not taken into account since the nucleus is considered to be at rest in the laboratory system. Further, the application of the free gas model to the resonant scattering of neutrons shows that the up-scattering probability is strongly dependent on the incident neutron energy. If the latter is smaller than the resonance energy then the free gas model predicts an enormous chance for the neutron to gain energy after collision.

Neither the static nor free gas model is adequate to describe the resonant scattering of neutrons in a crystal. This fact can induce non-negligible errors in reactor calculations and, in particular, in the estimation of the Doppler coefficient. In present paper we propose the theoretical study of the possibility to estimate the neutron transfer cross sections in the harmonic crystal approximation.

I. INTRODUCTION

In the present paper I propose an approximation which takes into account the influence of crystalline binding on the resonant scattering of neutrons. This approximation is based on the well-known short nucleus lifetime expansion (SNL), analogous to that first proposed by Wick[1] in the case of thermal-neutron scattering. Trammell[2] considered the application of SNL to the resonant scattering of neutrons in the case of the elastic scattering. A similar expansion can be applied to the inelastic[*] scattering of neutrons in a resonance.

The general expression for the resonant part of the transfer cross section (RTCS) taking into account the influence of chemical binding was derived by Word and Trammell.[3] It is

[*] In the rest of the paper the term 'inelastic' means that the final neutron state is different from its initial state. In consequence the final crystal state is altered from its initial state.

appropriate to display their result with a modification, which consists of considering the explicit dependence of the RTCS on the incident neutron energy:[4]

$$\frac{d^2\sigma_R}{d\Omega dE} = \frac{\upsilon}{2\pi}\left(\frac{\Gamma}{2k_i}\right)\left(\frac{E_f}{E_i}\right)^{1/2}\int_{-\infty}^{\infty} dT\exp(-iET)\int_0^{\infty} dt\exp[a(t)]\int_0^{\infty} dt'\exp[a^*(t')]\,W(T,t,t')$$

$$W(T,t,t') = \left\langle \exp\left[-i\vec{k}_i\vec{r}(T-t')\right]\exp\left[i\vec{k}_f\vec{r}(T)\right]\exp\left[-i\vec{k}_f\vec{r}\right]\exp\left[i\vec{k}_i\vec{r}(-t)\right]\right\rangle, \quad (1)$$

with $a(t) = -i(E_r - E_i - i\Gamma/2)t$.

In this expression the triangular brackets indicate that the thermal average over initial crystal states must be calculated. In the last formula the following notation is introduced: $\vec{k}_i$ and $\vec{k}_f$ - initial and final state neutron wave vectors, E_i and E_f - neutron energies before and after collision, E_r - level energy of compound nucleus; Γ - total width of the resonance; Γ_n - neutron width of the resonance; $\vec{r}$ - displacement of the nucleus in the Heisenberg's representation as a function of time, υ - factor taking into account the spin dependence of the interaction (statistical factor). All these quantities are given in the laboratory system. Here, and in the following discussion, I assumed the natural unit system where $\hbar = 1$. The variables t and t' are compound nucleus lifetimes, and T is the crystal interaction time. It is also assumed that the nuclear interaction can be satisfactorily described by single level Breit-Wigner's formalism. In calculating the last formula, the incoherent approximation[5] is used. In this approximation the interference effects from different sites in a crystal are neglected. This is a fair approximation in the resonance domain of heavy isotopes.

The quantity W is the correlation function, which is analogous to that of thermal-neutron scattering. In this work I focus on the harmonic crystal model in describing the atomic displacements. In this particular case, the Bloch theorem[5] can be used to estimate the thermal average in the function W. The result is:

$$W(T,t,t') = \exp\left\{-\left\langle\left(\vec{k}_i\vec{r}\right)^2\right\rangle - \left\langle\left(\vec{k}_f\vec{r}\right)^2\right\rangle\right\}\times\exp\left\{\left\langle\vec{k}_i\vec{r}(-t')\vec{k}_f\vec{r}\right\rangle + \left\langle\vec{k}_f\vec{r}\vec{k}_i\vec{r}(-t)\right\rangle\right\}\times$$
$$\times\exp\left\{-\left\langle\vec{k}_i\vec{r}(T-t')\vec{k}_f\vec{r}\right\rangle + \left\langle\vec{k}_i\vec{r}(T-t')\vec{k}_i\vec{r}(-t)\right\rangle + \left\langle\vec{k}_f\vec{r}(T)\vec{k}_f\vec{r}\right\rangle - \left\langle\vec{k}_f\vec{r}(T)\vec{k}_i\vec{r}(-t)\right\rangle\right\}. \quad (2)$$

It is hence seen that W is a product of three factors. The first exponential factor in the last expression does not depend on times. This factor provides an attenuation of the resonant process which is influenced by temperature and binding effects. The second factor depends only on t and t'. These two describe the contribution of virtual phonons created (absorbed) at the beginning of interaction and reabsorbed (remitted) at the end of the interaction. Finally, the variable T governs the exchange of real phonons. The third factor is a coupling between the nuclear process and the crystal dynamics.

This third factor introduces many difficulties to the numerical evaluation of the RTCS. In practice reactor physicists are interested in cross sections of heavy isotopes, such as uranium and plutonium. The low-lying resonances of these isotopes, which are of great importance in reactor applications, are not very large. Hence, the nuclear lifetimes t and t' vary between very and medium fast. In this situation it is convenient to make use of a truncated power series

representation of the correlation function W. I propose here to study the application of such an approach to resonant neutron scattering.

II. UNCOUPLED PHONON APPROXIMATION (UPA)

Trammell[2] considered the domain of short collision times in developing a model for the elastic scattering of neutrons in a resonance. His method can be applied to the inelastic scattering of neutrons in a resonance. Under the condition analogous to that introduced by Trammell:

$$\left| \Delta + R + i\left[\Gamma/2 + 2\sqrt{R\Theta}\right] \right| >> \omega_m, \quad \Delta = E_r - E_i, \tag{3}$$

the arguments of the first two exponential factors in W can be developed in power series about t, t'=0. Under the same condition one can neglect the dependence of the 'crossing' third exponential factor in (2) on t and t'. In the last expression I introduced the following notation: $R = \vec{k}_i\vec{k}_f / 2M$ - recoil energy of the nucleus, $\Theta = \int_0^\infty f(\omega)\omega \coth\frac{\omega}{2kT_c}d\omega$ - average energy of thermal vibrations per degree of freedom, ω_m - the characteristic frequency of atoms' vibrations, and T_c – thermodynamic crystal temperature.

By neglecting the dependence of the 'crossing' factor in (2) on t and t ' we uncouple somewhat the nuclear process from the crystal dynamics: that explains the term Uncoupled Phonon Approximation. Now we can calculated the contribution to the transfer cross section from t and t' separately. In terms of the function

$$Z(y) = \int_{-\infty}^{\infty} \frac{\exp(-t^2)}{y - t}dt,$$

the final result is:

$$\frac{d^2\sigma_R}{dEd\Omega} = \frac{\upsilon}{2\pi}\left(\frac{\Gamma_n}{2k_i}\right)^2\left(\frac{E_f}{E_i}\right)^{1/2}\int_{-\infty}^{\infty} dT \exp(-iET)\left\langle \exp\left[-i\Delta\vec{k}\vec{r}(0)\right]\exp\left[i\Delta\vec{k}\vec{r}(T)\right]\right\rangle \times \sigma_R^{UPA}, \tag{4}$$

with

$$\sigma_R^{UPA} = \begin{cases} \frac{1}{4\pi|R|\Theta} Z\left(\frac{\Gamma/2}{\sqrt{4|R|\Theta}}, \frac{\Delta - |R|}{\sqrt{4|R|\Theta}}\right) \times Z^*\left(\frac{\Gamma/2}{\sqrt{4|R|\Theta}}, \frac{\Delta - |R|}{\sqrt{4|R|\Theta}}\right), & R < 0 \\ \frac{1}{\Delta^2 + \Gamma^2/4}, & R = 0 \\ \frac{1}{4\pi|R|\Theta} Z\left(\frac{\Delta + R}{\sqrt{4R\Theta}}, \frac{\Gamma/2}{\sqrt{4R\Theta}}\right) \times Z^*\left(\frac{\Delta + R}{\sqrt{4R\Theta}}, \frac{\Gamma/2}{\sqrt{4R\Theta}}\right), & R > 0 \end{cases}$$

where $\Delta\vec{k} = \vec{k}_i - \vec{k}_f$. The preceding formula describes explicitly the Doppler effect, which relates to the recoil of the nucleus R and the broadening of the resonance width through the quantity $2\sqrt{R\Theta}$. The last formula gives the final expression for the RTCS for heavy nuclei in the resonance domain.

The expression for the interference term in the transfer cross section (ITCS) can be obtained in the same manner.

$$\frac{d^2\sigma_{int}}{dEd\Omega} = \upsilon \frac{\Gamma_n}{2k_i\pi}\left(\frac{E_f}{E_i}\right)^{1/2} \sqrt{\left(a^{coih}\right)^2 + \left(a^{incoh}\right)^2} \times \int_{-\infty}^{\infty} dT \exp(-iET)\left\langle \exp\left[-i\Delta\vec{k}\vec{r}(0)\right]\exp\left[i\Delta\vec{k}\vec{r}(T)\right]\right\rangle \times \sigma_{int}^{UPA}, \quad (5)$$

with

$$\sigma_{int}^{UPA} = \begin{cases} \dfrac{1}{\sqrt{4\pi|R|\Theta}}\,\mathrm{Im}\left[Z\left(\dfrac{\Gamma/2}{\sqrt{4|R|\Theta}}, \dfrac{\Delta - |R|}{\sqrt{4|R|\Theta}}\right)\right], & R < 0 \\ -\dfrac{\Delta}{\Delta^2 + \Gamma^2/4}, & R = 0 \\ \dfrac{1}{\sqrt{4\pi|R|\Theta}}\,\mathrm{Re}\left[-Z\left(\dfrac{\Delta + R}{\sqrt{4R\Theta}}, \dfrac{\Gamma/2}{\sqrt{4R\Theta}}\right)\right]. & R > 0 \end{cases}$$

Combining the results for the RTCS and ITCS with VanHove's result for thermal neutrons scattering[6] we can perform a calculation of the transfer cross section of heavy nuclei in the resonance domain.

Let me consider the domain of the validity of the UPA, which is given by the expression (3). This condition must be investigated for each particular application. As an example, let me consider the resonant scattering of neutrons from uranium ^{238}U nucleus bounded in its dioxide UO_2.

The total width of the first resonance of ^{238}U at E_Γ = 6.674 eV is $\Gamma/2$ = 0.01225 eV. The characteristic frequency of the uranium's atoms vibrations in UO_2 is $\omega_m \approx 0.011$ eV, and $\Theta \approx 0.027$ eV for the thermodynamic crystal temperature T_c=300K. First, if the total resonance width is not large then in the case where the energy of the incident neutron is far enough from the peak of the resonance ($|E_r - E_i| >> \omega_m$), UPA is a good approximation. Second, for the incident neutron energies close to the resonance peak, the validity condition of the UPA is strongly dependent on the scattering angle and is mostly determined by the natural width of the resonance. At high neutron energies, where resonance widths are larger, UPA can be considered as a good approximation in all energy range near the peak of the resonance.

III. CONCLUSION

The purpose of this paper is to describe a formalism that allows to take into account crystalline binding in the inelastic resonant scattering of neutrons. The Uncoupled Phonons Approximation has been developed on the basis of the earlier work of Trammell[2] on the elastic scattering of neutrons. This formalism enables to readily perform calculations of transfer cross section for heavy isotopes in the resonance domain and, consequently, to show the basic difference between the commonly used static model and a more realistic description of the resonant scattering of neutrons. Future work will be dedicated to the application of that formalism to the calculation of the transfer cross sections in the harmonic crystal model.

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