

COHERENT PRODUCTION OF COMPOUND NUCLEAR RESONANCES BY COLD NEUTRONS

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Dedicated to Adam Sobiczewski in honour of his 70th birthday

We consider the capture of a cold neutron (kinetic energy $< 0,1$ meV) by a crystal in the case that, at first, by the emission of a phonon, the neutron is absorbed by one of the lattice nuclei forming a compound nuclear resonance. Subsequently, the resonance decays by the emission of a photon. The energy of the compound nuclear resonance must be very close to the neutron threshold, *i.e.* within the range of phonon energies ($\lesssim 100$ meV), thus implying that the absorbing nuclei must be heavy actinides. We discuss the dependence of the capture process on the initial occupation pattern of phonons and, in particular, a mechanism of enhancing the absorption process.

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1. Introduction

Cold neutrons with a kinetic energy E below 10^{-1} meV (10^{-3} meV) have a de Broglie wavelength λ larger than 10 \AA (95 \AA). Whenever the neutron-wavelength is much larger than the interatomic distance in a crystal, neutrons which are scattered from nuclei of the same species, but at different sites of the crystal, interfere coherently. In particular, inelastic scattering of low energy neutrons which is correlated with the absorption or emission of phonons, plays a very important role for the study of the phonon spectrum of solids and liquids.

The theory of this process has been elegantly formulated by van Hove [?] and Glauber [?] in terms of space-time correlation functions using Born approximation in connection with Fermi's quasi-potential [?]. Whereas a huge amount of work has ever since been dedicated to the coherent scattering

of slow neutrons in solids, the *coherent absorption of neutrons* by the nuclei of the solid has received less attention, although Lamb [?], in an early and important theoretical paper, had drawn attention to this process.

In this note we reinvestigate this problem in the specific case of the absorption of cold neutrons by a crystal consisting entirely or partly of heavy actinide nuclei (N, Z) with N neutrons and Z protons.

If a neutron is absorbed by such a nucleus, the compound nuclear resonances of the $(N + 1, Z)$ system at excitation energies close to the neutron threshold E_{th} (\approx (5–8) MeV) have an average spacing $\langle D \rangle$ of (10–15) eV and an average width $\langle \Gamma \rangle \approx$ (10 to 30) meV. Let us assume that there is at least one such compound nuclear resonance at an energy $E_{\text{th}} - \Delta E_{\kappa}$ where $\Delta E_{\kappa} > 0$ is within the energy range of acoustic (\lesssim 30 meV) or of optical phonons (\lesssim 100 meV). In this case, a cold neutron of momentum \vec{p}_n may be absorbed forming this compound state by emission of a phonon of wave number \vec{q}_0 and of energy $E_{\text{ph}} = \hbar\omega_{\text{ph}}(\vec{q}_0)$.

As the wavelength $\lambda = \frac{\hbar}{p_n}$ of the incident neutron is supposed to be much larger than the distance between neighbouring (N, Z) -nuclei of the lattice, the compound nucleus $(N + 1, Z)^*$ may be anywhere in the crystal. In other words, the absorption of the neutron produces an excited state of the crystal where one target nucleus (N, Z) at any position \vec{R}_{α} of the lattice is replaced by the compound nucleus $(N + 1, Z)^*$. The formation amplitudes carry the phase $e^{i\vec{k}_n \cdot \vec{R}_{\alpha}/\hbar}$ (see Eq. (45)).

The compound nuclear resonance decays in turn either by γ -emission or by fission. It depends on the actinide nuclei in the crystal whether the fission channel is open or not. Usually, the fission channel is closed for even N and it may be open for odd N .

In any case, the physically interesting aspect is that the decay of the compound nuclei of the lattice occur *coherently* whenever they were produced by emission of a well-defined phonon. In what follows, we shall consider the case that the compound nuclei can only decay by emission of photons.

We present the theory in paragraph 2 and a discussion of the results and of open questions in paragraph 3.

2. Theory

The first question is: What is the Hamiltonian of the system “neutron plus crystal”? Let us denote the equilibrium positions of the lattice by \vec{R}_{α}^0 and let us assume, for the sake of formal simplicity, that the lattice contains only one type of nuclei with N neutrons and Z protons ($A := N + Z$).

Let us denote the vectors defining the centre of mass of the α -th atom by \vec{R}_{α} with the understanding that \vec{R}_{α} deviates from the equilibrium position \vec{R}_{α}^0 only slightly, *i.e.* by much less than the average distance “ a ” between

neighbouring lattice sites

$$|\vec{R}_\alpha - \vec{R}_\alpha^0| \ll a. \tag{1}$$

Each constituent nucleus of the crystal is supposed to consist of N neutrons and Z protons. The Z electrons of the lattice atoms will be left away because their interaction with the incoming neutron is small and their interactions with the radiation field plays no role in the process we consider. The number of crystal atoms is denoted by \mathcal{N} . For the sake of formal clarity, we treat the incoming neutron as distinguishable from the neutrons in the lattice nuclei. Furthermore, we treat nucleons which are localized in different nuclei of the lattice as distinguishable. Both these assumptions can be easily avoided, but they clarify the structure of the Hamiltonian.

Let us denote the position vector of the i -th nucleon in the α -th nucleus by \vec{x}_α^i , its spin and isospin variables by ζ_α^i and η_α^i , and the *relative* position vector with respect to the mass centre \vec{R}_α of the α -th nucleus by

$$\vec{x}_\alpha^{i'} = \vec{x}_\alpha^i - \vec{R}_\alpha. \tag{2}$$

Latin superscripts ($i, j, k \dots$) go from 1 to A and Greek subscripts ($\alpha, \beta, \gamma \dots$) from 1 to \mathcal{N} if not noted otherwise. The relative position vectors $\vec{x}_\alpha^{i'}$ have to satisfy the relations

$$\sum_{i=1}^A \vec{x}_\alpha^{i'} = 0 \tag{3}$$

due to the definition of \vec{R}_α . For the sake of simplicity, we shall neglect the constraints (3), *i.e.* we shall treat the relative position vectors $\vec{x}_\alpha^{i'}$ as independent variables. The Hamiltonian $\hat{\mathcal{H}}$ which describes the crystal consisting of \mathcal{N} nuclei (N, Z), the additional neutron with position vector \vec{x} and spin variable ζ , and the radiation field \hat{A} acting on the protons, can be written in the form

$$\hat{\mathcal{H}} = \sum_{\alpha=1}^{\mathcal{N}} \{ \hat{H}_\alpha + \hat{U}_\alpha \} + \frac{\hat{p}_n^2}{2M} + H_{\text{latt}}(\vec{R}_1 \dots \vec{R}_{\mathcal{N}}), \tag{4}$$

where $\hat{U}_\alpha(\vec{x} - \vec{R}_\alpha)$ is the sum of 2-body interactions between the additional neutron and the nucleons of the α -th nucleus

$$\hat{U}_\alpha(\vec{x} - \vec{R}_\alpha) := \sum_{i=1}^A v(\vec{x} - \vec{x}_\alpha^i; \zeta, \zeta_\alpha^i, \eta_\alpha^i) = \sum_{i=1}^A v(\vec{x} - \vec{x}_\alpha^{i'} - \vec{R}_\alpha; \zeta, \zeta_\alpha^i, \eta_\alpha^i) \tag{5}$$

\hat{p}_n and M are the momentum operator and the mass of the neutron, and \hat{H}_α is the Hamiltonian of the α -th nucleus including the coupling of the protons

to the radiation field \hat{A}

$$\hat{H}_\alpha(A) = \sum_{i=1}^A \left[\frac{\left(\hat{P}_\alpha^i - \frac{e_0}{c} \hat{A}(\vec{x}_\alpha^i)\right)^2}{2M} \hat{\tau}_p(\eta_\alpha^i) + \frac{\hat{p}_\alpha^{i2}}{2M} \hat{\tau}_n(\eta_\alpha^i) \right] + \sum_{i < j} v(\vec{x}_\alpha^i - \vec{x}_\alpha^j, \zeta_\alpha^i, \eta_\alpha^i, \zeta_\alpha^j, \eta_\alpha^j) + \sum_{\substack{i,j=1,\dots,A \\ i < j}} \frac{e_0^2}{|\vec{x}_\alpha^i - \vec{x}_\alpha^j|} \hat{\tau}_p(\eta_\alpha^i) \hat{\tau}_p(\eta_\alpha^j). \quad (6)$$

In Eq. (6), $\hat{\tau}_p$ and $\hat{\tau}_n$ are projection operators on protons and neutrons, respectively. The nuclear interaction between nucleons in different nuclei of the lattice is left away because it is negligible at normal densities of a crystal.

The last term $\hat{H}_{\text{latt}}(\vec{R}_1, \dots, \vec{R}_N)$ in Eq. (4) represents the Hamiltonian of the lattice vibrations, which consists of the kinetic energy of the nuclear mass centres and the Coulomb interaction $W(\vec{R}_1, \dots, \vec{R}_N)$ between the atoms¹.

$$\hat{H}_{\text{latt}} = \sum_{\alpha=1}^N \frac{\hat{P}_\alpha^2}{2M_\alpha} + W(\vec{R}_1, \dots, \vec{R}_N). \quad (7)$$

In Eq. (7), $\hat{P}_\alpha = \frac{\hbar}{i} \vec{\nabla}_{\vec{R}_\alpha}$ is the momentum operator conjugate to the mass center \vec{R}_α , and M_α is the mass of a crystal atom. The potential energy $W(\vec{R}_1, \dots, \vec{R}_N)$ of the ions has its minima at $\vec{R}_\alpha = \vec{R}_\alpha^0$. In the simplest approximation, one expands $W(\vec{R}_1 \dots \vec{R}_N)$ around $W(\vec{R}_1^0, \dots, \vec{R}_N^0)$ up to quadratic order. We use this “harmonic approximation” in what follows.

In Eqs (8) to (19), we present the introduction of phonon creation and annihilation operators in the simple case of a “linear chain”. The general case of a crystal containing several different atoms in a unit cell is treated extensively in the literature, for example in the references [?, ?, ?].

The linear chain consisting of one type of atoms is obtained by putting

$$\vec{R}_\alpha^0 = n \vec{a} = n a \vec{e}_x, \quad (8)$$

where \vec{a} is a vector in the direction of the linear chain with a length equal to the distance between neighbouring equilibrium positions of the lattice, and $n = 0, 1, 2, \dots$ are positive integers or 0. The vector \vec{e}_x is the unit vector in the direction of \vec{a} .

The deviation of atom α from its equilibrium position

$$\vec{u}_\alpha := \vec{R}_\alpha - \vec{R}_\alpha^0 \quad (9)$$

¹ We identify the charge centres with the mass centres of the atoms throughout this paper.

becomes simply

$$\vec{u}_\alpha = (R_\alpha - R_\alpha^0)\vec{e}_x = (R_\alpha - na)\vec{e}_x. \tag{10}$$

Assuming that the interaction acts only between nearest neighbours, the Hamiltonian \hat{H}_{latt} of the lattice assumes the form

$$\hat{H}_{\text{latt}} = \sum_{l=1}^{\mathcal{N}} \frac{\hat{p}_l^2}{2Ma} + \frac{f}{2} \sum_{l=1}^{\mathcal{N}-1} (\hat{u}_{l+1} - \hat{u}_l)^2 + \frac{1}{2} f (\hat{u}_{\mathcal{N}} - \hat{u}_1)^2, \tag{11}$$

where the parameter f is the spring constant and where cyclic boundary conditions

$$\hat{u}_{l+\mathcal{N}} = \hat{u}_l \tag{12}$$

are postulated.

It turns out that the solutions \hat{u}_n, \hat{p}_n can be written in the form [?]

$$\hat{u}_l = \hat{R}_{\text{CM}} + \sqrt{\frac{\hbar}{2Ma\mathcal{N}}} \sum'_q \frac{1}{\sqrt{\omega_q}} \left(\hat{b}_q e^{iqla} + \hat{b}_q^\dagger e^{-iqla} \right), \tag{13}$$

$$\hat{p}_l = \frac{1}{\mathcal{N}} \hat{P}_{\text{CM}} - i\sqrt{\frac{\hbar M_a}{2\mathcal{N}}} \sum'_q \sqrt{\omega_q} \left(\hat{b}_q e^{iqla} - \hat{b}_q^\dagger e^{-iqla} \right), \tag{14}$$

where the centre of mass variable \hat{R}_{CM} and its conjugate momentum \hat{P}_{CM} are defined by

$$\hat{R}_{\text{CM}} := \frac{1}{\mathcal{N}} \sum_{n=1}^{\mathcal{N}} \hat{u}_n, \tag{15}$$

$$\hat{P}_{\text{CM}} := \sum_{n=1}^{\mathcal{N}} \hat{p}_n \tag{16}$$

and where \hat{b}_q and \hat{b}_q^\dagger are annihilation and creation operators for phonons of energy

$$\hbar\omega_q = 2\hbar\omega_q \left| \sin \frac{qa}{2} \right| \tag{17}$$

satisfying Bose commutation relations.

The parameter q is defined to be

$$q = \frac{2\pi}{\mathcal{N}a} \kappa, \tag{18}$$

where² κ are \mathcal{N} consecutive non-zero integers varying between $-\frac{1}{2}(\mathcal{N} - 1)$ and $+\frac{1}{2}(\mathcal{N} - 1)$. The prime ' in Eqs (13), (14) means that $q = 0$ is to be omitted.

Introducing (13) and (14) into (11), we find that \hat{H}_{latt} becomes a sum of harmonic oscillators plus a kinetic energy of the mass centre:

$$\hat{H}_{\text{latt}} = \frac{\hat{P}_{\text{CM}}^2}{2M_a\mathcal{N}} + \sum_q' \hbar\omega_q \left(\hat{b}_q^\dagger \hat{b}_q + \frac{1}{2} \right). \quad (19)$$

For extended systems ($\mathcal{N} \rightarrow \infty$) at rest in the laboratory frame one may leave away \hat{R}_{CM} and $\frac{\hat{P}_{\text{CM}}}{\mathcal{N}}$ in Eqs (13) and (14), the *CM* energy $\frac{\hat{P}_{\text{CM}}^2}{2\mathcal{N}M_a}$ in Eq. (19) and the primes in the summations over q (see Ref. [?]).

In the general case of a 3-dimensional lattice, the harmonic Hamiltonian of a lattice with one atom in a unit cell reads [?]

$$\hat{H}_{\text{latt}} = \sum_{\vec{q}} \hbar\omega(\vec{q}) \left(\hat{b}_{\vec{q}}^\dagger \hat{b}_{\vec{q}} + \frac{1}{2} \right), \quad (20)$$

where, in generalization of Eq. (18), the wave vector \vec{q} of the phonon assumes all the values satisfying the condition

$$\vec{q}(\mathcal{N}_1\vec{a}_1 + \mathcal{N}_2\vec{a}_2 + \mathcal{N}_3\vec{a}_3) = 2\pi \text{ integer}. \quad (21)$$

Here, the vectors $\vec{a}_{1,2,3}$ define the primitive unit cell and $\mathcal{N}_{1,2,3}$ are the number of unit cells in the directions given by $\vec{a}_{1,2,3}$.

Let us now come to the coupling of the incoming neutron to the phonons and to the nucleons in the lattice nuclei:

$$\hat{H}_{n\text{-cryst}} := \sum_{\alpha=1}^{\mathcal{N}} \hat{U}_\alpha(\vec{x} - \vec{R}_\alpha) \quad (22)$$

with

$$\hat{U}_\alpha(\vec{x} - \vec{R}_\alpha) := \sum_{i=1}^A v(\vec{x} - \vec{x}_\alpha^i - \vec{R}_\alpha). \quad (23)$$

It provides the coupling of the additional neutron with the phonons of the lattice and, at the same time, with the nucleonic degrees of the nuclei. In Eq. (23) and, henceforward, we leave away the spin and isospin variables.

We draw attention to the fact that the interaction \hat{U}_α defined in (23) depends on the lattice location α only through the variable \vec{R}_α of the mass center, whereas its functional dependence is the same for all the α .

² Here, we assume \mathcal{N} to be odd. As \mathcal{N} is of the order 10^{23} , the limits are also valid for even \mathcal{N} .

Using (9) we have

$$\hat{U}_\alpha = \hat{U}(\vec{x} - \vec{R}_\alpha^0 - \hat{u}_\alpha). \tag{24}$$

Typical dislocations \hat{u}_α are in general not small compared to the nuclear radius and, therefore, contrary to the case of the electron-phonon coupling ([?, ?]), the linear approximation

$$\hat{U}(\vec{x} - \vec{R}_\alpha^0 - \vec{u}_\alpha) \approx \hat{U}(\vec{x} - \vec{R}_\alpha^0) - (\vec{\nabla}_y \hat{U}(\vec{y}))_{\vec{x} - \vec{R}_\alpha^0} \vec{u}_\alpha \tag{25}$$

may be occasionally insufficient.

At the same time, the so-called “adiabatic approximation”, *i.e.* the assumption that the velocity of lattice ions is much smaller than the velocity of the neutron, is no longer true for very cold neutrons. The velocity of a neutron with kinetic energy 1 meV (0,1 meV) is $4, 2 \times 10^{12}$ Å/s ($1, 3 \times 10^{12}$ Å/s) and the mean velocity of a ^{238}U -ion in a crystal of $k_B T = 1$ meV ($k_B T = 0, 1$ meV) is $0, 35 \times 10^{12}$ Å/s ($0, 1 \times 10^{12}$ Å/s). For an ^{16}O -ion the mean velocity at $k_B T = 1$ meV (0,1 meV) is $1, 3 \times 10^{12}$ Å/s ($0, 4 \times 10^{12}$ Å/s).

This means that the absorption of a cold neutron by formation of a compound nucleus embedded in a crystal may also occur together with the creation of more than one phonon (see Ref. [?]), which corresponds to higher order terms in Eq. (25).

The Hamiltonian \hat{H}_α of the α -th nucleus may be decomposed into the coupling $\hat{H}_\alpha^{p\gamma}$ of the protons to the radiation field \hat{A} and the remainder $\hat{H}_\alpha^{(0)}$:

$$\hat{H}_\alpha \approx \hat{H}_\alpha^{(0)} + \hat{H}_\alpha^{p\gamma}, \tag{26}$$

$$\begin{aligned} \hat{H}_\alpha^{(0)}(A) &= \sum_{i=1}^A \frac{\hat{p}_\alpha^i{}^2}{2M} + \sum_{i,j=1\dots A} v(\vec{x}_\alpha^i - \vec{x}_\alpha^j, \zeta_\alpha^i, \eta_\alpha^i, \zeta_\alpha^j, \eta_\alpha^j) \\ &+ \sum_{\substack{i,j=1\dots A \\ i < j}} \frac{e_0^2}{|\vec{x}_\alpha^j - \vec{x}_\alpha^i|} \hat{\tau}_p(\eta_\alpha^i) \hat{\tau}_p(\eta_\alpha^j), \end{aligned} \tag{27}$$

$$\hat{H}_\alpha^{p\gamma} = -\frac{e_0}{2Mc} \sum_{i=1}^A \left\{ \hat{p}_\alpha^i, \hat{A}(\vec{x}_\alpha^i) \right\} \hat{\tau}_p(\eta_\alpha^i), \tag{28}$$

where $\hat{p}_\alpha^i = \frac{\hbar}{i} \vec{\nabla}_{\vec{x}_\alpha^i}$, $M =$ nucleon mass, $e_0 =$ elementary charge. The photon-nucleus coupling $\hat{H}_\alpha^{p\gamma}$ leads to the decay of the compound nucleus formed in the vicinity of lattice position \vec{R}_α^0 by emission of a photon.

We are specially interested in a n -capture process where only 1 phonon is emitted, *i.e.* we want to consider the cross-section for the reaction

$$n + \{\mathcal{N}(N, Z)\} = \{(\mathcal{N} - 1)(N, Z) + (N + 1, Z)_{\text{res}}\} + \text{phonon}, \tag{29}$$

$$\{(\mathcal{N} - 1)(N, Z) + (N + 1, Z)_{\text{res}}\} \rightarrow \{(\mathcal{N} - 1)(N, Z) + (N + 1, Z)_f\} + \text{photon}. \quad (30)$$

Here, we denote the state of the crystal of \mathcal{N} atoms by $\{\}$, the compound nucleus at an energy close to the neutron threshold by $(N + 1, Z)_{\text{res}}$ and the (supposedly long-lived) final state of this nucleus after the γ -emission by $(N + 1, Z)_f$.

We assume one nuclear compound resonance $(N + 1, Z)_{\text{res}}$ of small total width Γ ($\Gamma \lesssim 1$ meV) to be so close to the n -threshold that an incoming cold neutron can be absorbed by the crystal of $\mathcal{N}(N, Z)$ nuclei by emission of a phonon (see Eq. (29)).

Of course, the compound nucleus $(N + 1, Z)_{\text{res}}$ can be located anywhere in the crystal. We assume that it decays by emission of a photon (see Eq. (28)) to a long-lived final state $(N + 1, Z)_f$.

A vibrational state of the crystal is defined by the set $\{n_{\vec{q}}\}$ of occupation numbers of all the possible phonon quasi-momenta \vec{q} . We denote the initial state of the lattice by $|\{n_{\vec{q}}^{(i)}\}\rangle$ and the final one by $|\{n_{\vec{q}}^{(f)}\}\rangle$. We consider the case that the incoming cold neutron is captured by the emission of *one* phonon of given wave-vector \vec{q}_0 . Thus the final and initial phonon occupation numbers are related to each other by

$$n_{\vec{q}}^{(f)} = n_{\vec{q}}^{(i)}(1 - \delta_{\vec{q}\vec{q}_0}) + (n_{\vec{q}_0}^{(i)} + 1)\delta_{\vec{q}\vec{q}_0}, \quad (31)$$

where the Kronecker symbol $\delta_{\vec{q}\vec{q}_0}$ is 1 for $\vec{q} = \vec{q}_0$ and otherwise zero.

The *initial state* of the system is denoted by

$$|i\rangle \equiv \left| \left\{ n_{\vec{q}}^{(i)} \right\}; \prod_{\delta=1}^{\mathcal{N}} \Psi(N, Z, \vec{R}_{\delta}); \vec{k}_n m_s \right\rangle, \quad (32)$$

where $\Psi(N, Z, \vec{R}_{\delta})$ is the groundstate of the (N, Z) -nucleus with mass centre at \vec{R}_{δ} , \vec{k}_n is the wave-vector of the incoming neutron, and m_s the magnetic spin quantum number of the neutron³.

The *intermediate states* of the system are characterized by the final phonon occupation numbers $\{n_{\vec{q}}^{(f)}\}$, the quantum numbers κ and the energy E_{κ}^* of the compound nucleus $(N + 1, Z)$ and the label λ which tells us that the mass centre \vec{R}_{λ} of the compound nucleus $(N + 1, Z)$ is distributed in the vicinity of the lattice site \vec{R}_{λ}^0 . We denote these states by

$$|R\lambda\rangle \equiv \left| \left\{ n_{\vec{q}}^{(f)} \right\}; \prod_{\substack{\delta'=1, \dots, \mathcal{N} \\ \delta' \neq \lambda}} \Psi(N, Z; \vec{R}_{\delta'}) \Psi_{\kappa}(N + 1, Z; \vec{R}_{\lambda}) \right\rangle. \quad (33)$$

³ The plane waves of the neutron and of the emitted photon are normalized to 1 in the effective volume L^3 of the crystal: $L^{-3/2} \exp[i\vec{k}_n \cdot \vec{x}]$ and $L^{-3/2} \exp[i\vec{k}_{\gamma} \cdot \vec{x}]$

Here, $\Psi_\kappa(N + 1, Z; \vec{R}_\lambda)$ is an excited state of the nucleus $(N + 1, Z)$ with mass centre \vec{R}_λ .

All the \mathcal{N} states (33) are energetically degenerate. $\Psi(N, Z; \vec{R}_\delta)$ is the groundstate of the Hamiltonian $\hat{H}_\delta(A)$ and $\Psi_\kappa(N + 1, Z; \vec{R}_\lambda)$ an excited state of the Hamiltonian $\hat{H}_\delta(A + 1)$ given by Eq. (6) with the nucleon number A replaced by $(A + 1)$.

The *final states* of the system are characterized by a γ -quantum of wave-vector \vec{k}_γ and polarization \mathcal{E}_γ , an excited $(N + 1, Z)$ -nucleus with mass centre position \vec{R}_λ specified by the quantum number β and the excitation energy E_{β_f} . All the states differing by the location of the excited $(N + 1, Z)$ -nucleus in the lattice are again degenerate. We denote the final states by

$$|f\rangle \equiv \left| \left\{ n_{\vec{q}}^{(f)} \right\} \prod_{\substack{\delta'=1 \\ \delta' \neq \lambda}}^{\mathcal{N}} \Psi(N, Z; \vec{R}_{\delta'}) \Psi_\beta(N + 1, Z; \vec{R}_\lambda), \vec{k}_\gamma \mathcal{E}_\gamma \right\rangle. \quad (34)$$

The reaction amplitude has the form of a sum of Breit–Wigner terms, each term corresponding to a specific location of the $(N + 1, Z)$ nucleus in the lattice and all terms with the same denominator:

$$\langle f | \hat{T} | i \rangle = \sum_{\lambda=1}^{\mathcal{N}} \frac{\Gamma_{f,R\lambda}^{1/2} \Gamma_{R\lambda,i}^{1/2}}{(E - E_\kappa - \hbar\omega_{\vec{q}_0}) - \frac{i}{2} \Gamma_\kappa}. \quad (35)$$

Here, E is the total energy of the system, E_κ is the energy of the system at resonance apart from the energy $\hbar\omega_{\vec{q}_0}$ of the phonon, and Γ_κ is the total width of the resonance⁴. The energies E and E_κ can be decomposed as follows

$$E = E_n + \mathcal{N} E(N, Z) + W(\vec{R}_1, \dots, \vec{R}_\mathcal{N}), \quad (36)$$

$$E_\kappa = E_\kappa^*(N + 1, Z) + (\mathcal{N} - 1)E(N, Z) + W(\vec{R}_1, \dots, \vec{R}_\mathcal{N}). \quad (37)$$

Here, $E(N, Z)$ is the groundstate energy of the nucleus (N, Z) , $E_\kappa^*(N + 1, Z)$ is the energy of the compound nucleus $(N + 1, Z)^*$, $E_n \gtrsim 0$ is the kinetic energy of the incoming neutron, and W is the electromagnetic potential energy of the crystal consisting of \mathcal{N} atoms. Introducing the threshold energy E_{th} for emission of a neutron from the nucleus $(N + 1, Z)$ (=“Ablösearbeit”)

$$E_{\text{th}} := E(N, Z) - E(N + 1, Z) \quad (38)$$

⁴ We use the laboratory reference frame where the crystal is initially at rest. Consequently, by the absorption of the neutron, the mass centre of the crystal acquires a recoil momentum \vec{P}^* which is related to a wave vector \vec{K}^* of the reciprocal lattice by $\vec{P}^* = -\hbar\vec{K}^*$ (see for instance Ref. [?]). The recoil energy $\vec{P}^{*2}/2M_{\text{cryst}}$ turns out to be extremely small because of the large mass of the crystal $M_{\text{cryst}} = \mathcal{N}M_{\text{atom}}$ and is, therefore, left away in the denominator of Eq. (35).

we may write $E_\kappa^*(N + 1, Z)$ in the form

$$E_\kappa^*(N + 1, Z) = E(N + 1, Z) + E_{\text{thr}} - \Delta E_\kappa, \quad (39)$$

where $\Delta E_\kappa > 0$ is the energy distance of the compound nuclear resonance from the neutron threshold of the $(N + 1, Z)$ nucleus. Using (36)–(39), the energy difference $(E - E_\kappa)$ can be written in the form

$$E - E_\kappa = E_n + \Delta E_\kappa. \quad (40)$$

In Eqs (36), (37), we neglected the tiny influence upon the electromagnetic energy W which is produced by replacing one of the \mathcal{N} nuclei (N, Z) of the crystal by a nucleus $(N + 1, Z)$. This approximation and the neglect of the recoil energy of the total mass centre (see footnote) are the reasons why the lattice dynamics enters the denominator of Eq. (35) only through the phonon energy $\hbar\omega_{\vec{q}_0}$.

The quantities $\Gamma_{R\lambda, i}$ and $\Gamma_{f, R\lambda}$ in the numerator of (35) represent the partial widths for the formation of the intermediate states $|R\lambda\rangle$ of the system from the entrance channel and for the decay of the intermediate states by emission of a γ -quantum. Assuming that these widths can be calculated by perturbation theory, they are given by

$$\Gamma_{R\lambda, i} = \left\langle \left\{ n_{\vec{q}}^{(f)} \right\}; \prod_{\substack{\delta'=1, \dots, \mathcal{N} \\ \delta' \neq \lambda}} \Psi(N, Z; \vec{R}_{\delta'}) \Psi_\kappa(N + 1, Z; \vec{R}_\lambda) \left| \hat{U}(\vec{x} - \vec{R}_\lambda) \right| \left\{ n_{\vec{q}}^{(i)} \right\}; \prod_{\delta=1, \dots, \mathcal{N}} \Psi(N, Z; \vec{R}_\delta); \vec{k}_n m_s \right\rangle \quad (41)$$

and by

$$\Gamma_{f, R\lambda} = \left\langle \left\{ n_{\vec{q}}^{(f)} \right\}; \prod_{\substack{\delta''=1, \dots, \mathcal{N} \\ \delta'' \neq \lambda}} \Psi(N, Z; \vec{R}_{\delta''}) \Psi_\beta(N + 1, Z; \vec{R}_\lambda); \vec{k}_\gamma \varepsilon_\gamma \left| \hat{H}_\lambda^{p\gamma} \right| \left\{ n_{\vec{q}}^{(f)} \right\}; \prod_{\substack{\delta'=1, \dots, \mathcal{N} \\ \delta' \neq \lambda}} \Psi(N, Z; \vec{R}_{\delta'}) \Psi_\kappa(N + 1, Z; \vec{R}_\lambda) \right\rangle. \quad (42)$$

Let us now study these matrix elements in more detail:

The eigenstate $\Psi_\kappa(N + 1, Z; \vec{R}_\alpha)$ is a normalized eigenstate with eigenenergy E_κ^* of the Hamiltonian $\hat{H}_\alpha^{(0)}$ (see (27)) where the nucleon number A is replaced by $(A + 1)$ due to the fact that the number of neutrons is $(N + 1)$ instead of N , whereas $\Psi(N, Z; \vec{R}_\alpha)$ is the groundstate of $\hat{H}_\alpha^{(0)}(A)$ as defined in (27).

The quantum numbers κ specifying the compound nuclear state contain the angular momentum j_{res} and its projection m_{res} . If the absorbing nucleus is an even-even nucleus with angular momentum 0, the compound nucleus has the angular momentum $j_\kappa = 1/2$ and the magnetic quantum number $m_\kappa = m_s$ of the absorbed cold neutron. If the absorbing nucleus is an odd or odd-odd nucleus with a finite angular momentum j_0 , the angular momentum j_κ of the compound nucleus may have the values ($j_0 \pm 1/2$) and corresponding values of the magnetic quantum number.

The spectrum of phonon wave vectors \vec{q} which is determined by the periodic boundary conditions of Eq. (21), must be cut off at an upper frequency limit which is reasonably chosen in such a way that the number of wave numbers agrees with $3\mathcal{N}$ where \mathcal{N} is the number of crystal atoms.

The total width Γ_κ of the intermediate states is the sum of the partial decay widths. Intermediate states which differ only by the location of the compound nucleus in the lattice have the same total width as subsumed in Eq. (35). The dominant decay widths are provided by γ -decay and possibly nuclear fission.

We note that nuclear wave functions localized around different lattice sites are practically orthogonal because the lattice constants $a_{1,2,3}$ exceed the nuclear radius by a factor of 10^4 :

$$\langle \Psi(N, Z, \vec{R}_\lambda) | \Psi(N, Z, \vec{R}_{\lambda'}) \rangle \approx \delta_{\lambda\lambda'}. \tag{43}$$

Up to a factor (see for instance Ref. [?]), the transition probability per time unit $W(\beta, \vec{k}_\gamma, \varepsilon_\gamma, \vec{q}_0; \vec{k}_n m_s)$ is given by the absolute square of the reaction amplitude defined in Eq. (35):

$$W_{fi}(\beta, \vec{k}_\gamma, \varepsilon_\gamma, \vec{q}_0; \vec{k}_n m_s) = \left(\frac{\pi \hbar}{M L^3 k_n} \right) \frac{\sum_{\lambda, \lambda'=1}^{\mathcal{N}} \Gamma_{f, R\lambda}^{1/2} \Gamma_{R\lambda, i}^{1/2} (\Gamma_{f, R\lambda'})^* (\Gamma_{R\lambda', i})^*}{(E - E_\kappa - \hbar\omega_{\vec{q}_0})^2 + \frac{1}{4} \Gamma_\kappa^2}. \tag{44}$$

When evaluating the partial widths $\Gamma_{R\lambda, i}$ and $\Gamma_{f, R\lambda}$ (see (41), (42)) the integrations over the nucleonic variables of the nuclei $\Psi(N, Z; \vec{R}_\delta)$ are trivial because of the orthonormality (43). In addition, it is easily seen that the matrix elements (41) and (42) factorize as follows

$$\begin{aligned} \Gamma_{R\lambda, i} &= \left\langle \left\{ n_{\vec{q}}^{(f)} \right\} \left| e^{i\vec{k}_n \cdot \vec{R}_\lambda} \left| \left\{ n_{\vec{q}}^{(i)} \right\} \right. \right\rangle \langle \Psi_\kappa(N + 1, Z) | \hat{\mathcal{U}} | \Psi(N, Z), \vec{k}_n m_s \rangle, \tag{45} \\ \Gamma_{f, R\lambda} &= \left\langle \left\{ n_{\vec{q}}^{(f)} \right\} \left| e^{-i\vec{k}_\gamma \cdot \vec{R}_\lambda} \left| \left\{ n_{\vec{q}}^{(f)} \right\} \right. \right\rangle \langle \Psi_\beta(N + 1, Z) \vec{k}_\gamma \varepsilon_\gamma | \hat{H}^{p\gamma} | \Psi_\kappa(N + 1, Z) \rangle. \tag{46} \end{aligned}$$

Here, the notation of the second factors implies that they do not depend on the label λ of the lattice site because \vec{R}_λ occurs only in the definition of the intrinsic variables $\vec{x}_\lambda^{i'} = \vec{x}_\lambda^i - \vec{R}_\lambda$, which are integrated over.

Taking over the notation of Ref. [?], we denote these factors by

$$M_{\text{comp}}(\vec{k}_n, m_s) := \langle \Psi_\kappa(N + 1, Z) | \hat{\mathcal{U}} | \Psi(N, Z), \vec{k}_n m_s \rangle, \tag{47}$$

$$M_{\text{rad}}(\vec{k}_\gamma, \varepsilon_\gamma, \beta, \kappa) := \langle \Psi_\beta(N + 1, Z) | \vec{k}_\gamma \varepsilon_\gamma | \hat{H}^{P\gamma} | \Psi_\kappa(N + 1, Z) \rangle. \tag{48}$$

Our occupation numbers $\{n_{\vec{q}}^{(i)}\}$ and $\{n_{\vec{q}}^{(f)}\}$ differ only by one specific occupation number $n_{\vec{q}_0}^{(f)} = n_{\vec{q}_0}^{(i)} + 1$.

It should, however, be noted that the operators $e^{i\vec{k}_n \vec{u}_\lambda}$ and $e^{-i\vec{k}_\gamma \vec{u}_\lambda}$ have also non-vanishing matrix elements between states of the lattice which differ by more than 1 phonon. If one were to take such multiple phonon processes into account, one would have to sum in Eq. (35) not only over the lattice sites λ but also over the phonon occupation patterns $\{n_{\vec{q}}\}$ which may occur as intermediate states. We note that this was done in Ref. [?] which is the work this paper is based on, but with the result that one phonon creation and annihilation processes do give the most important contribution.

On the other hand, in Ref. [?], W. Lamb did not include a summation over all the lattice sites λ in (35) arguing that the neutron is absorbed by one definite nucleus λ of the lattice and that the resulting absorption probability did not depend on which one.

In what follows we shall see under which conditions our more general treatment yields the result of Ref. [?]: Substituting (45)–(47) into (44) and averaging at the same time over initial phonon occupation patterns with a weight function $w(\{n_{\vec{q}}^{(i)}\})$ we obtain the average transition probability W

$$\begin{aligned} W(\beta, \vec{k}_\gamma, \varepsilon_\gamma, \vec{q}_0; \vec{k}_n m_s) &= \left(\frac{\pi \hbar}{ML^3 k_n} \right) \\ &\times \frac{1}{[(E - E_\kappa - \hbar\omega_{\vec{q}_0})^2 + 1/4\Gamma_\kappa^2]} \sum_{\{n_{\vec{q}}^{(i)}\}} w(\{n_{\vec{q}}^{(i)}\}) \\ &\times \left\{ \sum_{\lambda=1 \dots \mathcal{N}} |\Gamma_{f,R\lambda}| |\Gamma_{R\lambda,i}| + \sum_{\substack{\lambda, \lambda'=1 \dots \mathcal{N} \\ \lambda \neq \lambda'}} \Gamma_{f,R\lambda}^{1/2} \Gamma_{f,R\lambda'}^{1/2*} \Gamma_{R\lambda,i}^{1/2} \Gamma_{R\lambda',i}^{1/2*} \right\}. \tag{49} \end{aligned}$$

We call the term with $\lambda = \lambda'$ the “incoherent” and the term with $\lambda \neq \lambda'$ the “coherent” contribution.

Introducing the dislocations \vec{u}_α (see Eq. (9)), the phonon matrix-elements can be written

$$\left\langle \left\{ n_{\vec{q}}^{(f)} \right\} \left| e^{i\vec{k}_n \vec{R}_\lambda} \left| \left\{ n_{\vec{q}}^{(i)} \right\} \right. \right\rangle = e^{i\vec{k}_n \vec{R}_\lambda^0} \left\langle \left\{ n_{\vec{q}}^{(f)} \right\} \left| e^{i\vec{k}_n \vec{u}_\lambda} \left| \left\{ n_{\vec{q}}^{(i)} \right\} \right. \right\rangle, \tag{50}$$

$$\left\langle \left\{ n_{\vec{q}}^{(f)} \right\} \left| e^{-i\vec{k}_\gamma \vec{R}_\lambda} \left| \left\{ n_{\vec{q}}^{(f)} \right\} \right\rangle = e^{-i\vec{k}_\gamma \vec{R}_\lambda^0} \left\langle \left\{ n_{\vec{q}}^{(f)} \right\} \left| e^{-i\vec{k}_\gamma \vec{u}_\lambda} \left| \left\{ n_{\vec{q}}^{(f)} \right\} \right\rangle. \quad (51)$$

Matrix-elements of the type $\langle \{n_{\vec{q}}^{(1)}\} | e^{i\vec{Q}\vec{u}_\lambda} | \{n_{\vec{q}}^{(2)}\} \rangle$ where $\{n_{\vec{q}}^{(1)}\}, \{n_{\vec{q}}^{(2)}\}$ are two arbitrary occupation patterns of phonons and \vec{Q} is some wave vector can be evaluated in closed form (see for instance Ref. [?], chapt. 8 and also Ref. [?]).

In the coherent part of the transition probability W , the main dependence on the lattice sites is produced by the factors $e^{i(\vec{k}_n - \vec{k}_\gamma)(\vec{R}_\lambda^0 - \vec{R}_{\lambda'}^0)}$. Substantial coherence effects from reactions occurring at different lattice sites can only arise if, for a large number of terms $\lambda \neq \lambda'$, the exponent $(\vec{k}_n - \vec{k}_\gamma)(\vec{R}_\lambda^0 - \vec{R}_{\lambda'}^0)$ varies slowly as a function of the momentum difference $(\vec{p}_n - \vec{p}_\gamma)$. This is the case when both the momenta $\vec{p}_n = \hbar\vec{k}_n$ and $\vec{p}_\gamma = \hbar\vec{k}_\gamma$ correspond to de Broglie wavelengths λ_n and λ_γ which are of the order of the lattice spacing or larger. This is the case for neutron energies $E_n < 0.1$ meV and for γ -decay energies $p_\gamma c \gtrsim < 10$ keV. As the decaying compound nuclear resonance has an energy of (5–8) MeV, rapid γ -decays in the MeV range, for which there is no coherent contribution, dominate the decay. Of course, the density of levels at an excitation energy of (5–8) MeV is so large that there are many γ -decay channels with $p_\gamma c \lesssim 10$ keV. Unfortunately, the transition strength of such low-energy transitions is very tiny.

In the usual case where only the incoherent part of (49) need be considered, the contributions $|I_{f,R\lambda}| |I_{R\lambda,i}|$ depend weakly on λ which brings us back to the case treated in Ref. [?]:

$$\begin{aligned} |I_{f,R\lambda}| |I_{R\lambda,i}| &= |M_{\text{comp}}(\vec{k}_n, m_s)| |M_{\text{rad}}(\vec{k}_\gamma, \varepsilon_\gamma, \beta, \kappa)| \\ &\times \left| \left\langle \left\{ n_{\vec{q}}^{(f)} \right\} \left| e^{-i\vec{k}_\gamma \vec{u}_\lambda} \left| \left\{ n_{\vec{q}}^{(f)} \right\} \right\rangle \right| \left| \left\langle \left\{ n_{\vec{q}}^{(f)} \right\} \left| e^{i\vec{k}_n \vec{u}_\lambda} \left| \left\{ n_{\vec{q}}^{(i)} \right\} \right\rangle \right|. \end{aligned} \quad (52)$$

If the crystal is at a temperature T , the weight factors $w(\{n_{\vec{q}}^{(i)}\})$ are given by the Boltzmann factor

$$w\left(\left\{n_{\vec{q}}^{(i)}\right\}\right) = \frac{\exp\left[-\frac{E(\{n_{\vec{q}}^{(i)}\})}{k_B T}\right]}{Z}, \quad (53)$$

where Z is the partition function.

Apart from the matrix elements M_{comp} and M_{rad} , the cross section may be evaluated in closed form. The calculation proceeds in a similar way as for inelastic neutron scattering (see Ref. [?], chapt. 8.4) and similarly to the one in Ref. [?]. There, a summation over the final γ -decays and over the phonon occupation patterns has been performed which excludes a coherent distribution altogether.

3. Discussion

The present paper differs from the basic work of Ref. [?] in two respects: The final states are not summed over and we assume that *one specific phonon* is emitted instead of many. Consequently, a coherent contribution to the transition rate appears which vanishes in Ref. [?]. As we have pointed out, interferences from decays of the coherently produced compound nuclear resonances can in principle be observed, but only under rather exceptional conditions. One of these conditions is, of course, that at least one sort of the nuclei in the crystal exhibit a compound nuclear resonance at an energy ΔE_κ below the neutron threshold E_{thr} with ΔE_κ in the range of phonon energies. This is a fortunate accident, which is, however, not impossible in the case of actinide nuclei.

One may envisage still another aspect of the system investigated:

Let us suppose that the weights $w(\{n_{\vec{q}}^{(i)}\})$ are not simply given by the Boltzmann factor but that they are specifically high for an interval of phonon energies around $\hbar\omega(\vec{q}_0)$, and of phonon wave vectors \vec{q} close to \vec{q}_0 . This would mean that the phonon which is emitted in the capture process is already present in the initial state of the crystal with a high occupation number $n_{\vec{q}_0}^{(i)} \gg 1$. In our case, *i.e.* for the occupation pattern defined in Eq. (31), the matrix-element $\langle \{n_{\vec{q}}^{(f)}\} | e^{i\vec{k}_n \vec{u}_\lambda} | \{n_{\vec{q}}^{(i)}\} \rangle$ turns out to be *proportional* to $\sqrt{n_{\vec{q}_0}^{(i)}}$. Thus, the probability of capture of the neutron into the resonant state $\Psi_\kappa(N+1, Z)$ by emission of a phonon would be enhanced by the factor $n_{\vec{q}_0}^{(i)}$.

Unfortunately, it is difficult to judge whether it is experimentally possible to produce a non-thermal initial occupation pattern. Neglecting the recoil of the entire crystal, the conservation of energy (up to width Γ_κ) and momentum

$$E_n + \Delta E_\kappa = \hbar\omega_{\vec{q}}, \quad (54)$$

$$\hbar\vec{k}_n = \hbar\vec{q}_0 \quad (55)$$

tell us that the emitted phonon would have to be an *optical phonon*. In the case of $E_n = 1$ meV (10 meV) one has $k_n = 0, 476 \text{ \AA}^{-1}$ ($1, 5 \text{ \AA}^{-1}$). A typical phonon energy would be $\hbar\omega_{\vec{q}_0} = 50$ meV. Optical phonons can in principle be produced by free electron lasers in materials with a sufficiently large dipole polarizability. Perhaps uranium oxyde would be such a material.

Due to phonon-phonon interactions, which come about by 3rd and 4th order terms in the expansion of $W(\vec{R}_1 \dots \vec{R}_N)$, the optical phonons decay with an average lifetime of 10^{-12} s. This lifetime would still be larger by a factor of 10 to 100 than the lifetime of a compound resonance of a heavy actinide

nucleus [8]. Thus it is permissible to calculate the transition-probability assuming a stationary initial phonon population as we have done.

Assuming that a large absorption rate can be experimentally achieved and that the compound resonance may decay with a not too unfavourable branching ratio into a long-lived nuclear isomer, one can dream to use the capture of cold neutrons as a pumping mechanism:

At high flux reactors, a flux $j_{\text{cold } n}$ of cold neutrons of the order of $(1-5) \times 10^{14} [\frac{n}{\text{cm}^2\text{s}}]$ can be reached. If the beam impinges perpendicularly upon a surface ΔF of the crystal and if the length of the crystal in the direction of the incoming neutrons is L , the average number of cold neutrons in the effective volume of the crystal is given by $\{j_{\text{cold } n} \Delta F \frac{L}{v_n}\}$ where v_n is the velocity of the neutron. The product

$$N^* = j_{\text{cold } n} \Delta F L \frac{W}{v_n} \quad (56)$$

represents the number of final nuclei produced per time unit by a specific (n, γ) reaction. W is the transition probability (49). At modern high flux reactors, one can attain cold neutron flux densities $j_{\text{cold } n}$ of about $3 \times 10^{14} [1/\text{cm}^2\text{s}]$ for $E_n < 10$ meV, $6 \times 10^{13} [1/\text{cm}^2\text{s}]$ for $E_n < 1$ meV, and $1, 2 \times 10^{13} [1/\text{cm}^2\text{s}]$ for $E_n < 0, 1$ meV.

This paper, which I dedicate to Adam Sobiczewski on the occasion of his 70th birthday, involves knowledge from fields of research where I am not an expert. I am particularly grateful to all the colleagues who have sacrificed time to instruct me, especially Gilbert Belier (Centre d'Etudes de Bruyères), and Franz von Feilitzsch, Joachim Hartmann and Peter Vogl (Physics Department of the TUM).

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