Neutron Bands in Solids

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Abstract

Low energy neutrons in a crystal behave as a wave and a band structure appears in the energy spectrum of the neutrons. A preliminary band calculation is given for a neutron in a one-dimensional Kronig-Penny lattice using the Fermi quasi-potential for the interaction between the neutron and lattice nuclei. It is suggested that a neutron in a band state of a crystal surrounded by others with a different band structure might be trapped in the crystal and the neutron might be responsible for new phenomena in solids.

1. Introduction

Low energy neutrons with a de Broglie wave length comparable with lattice constants are widely used as a tool for structural analysis of matter[1,2]. Characteristic behaviors of neutrons have been investigated in recent decades.

The neutrons interacting with nuclei bound in crystals (lattice nuclei)[3,4] have exhibited a similar feature of interaction with individual nucleus as in vacuum (free nucleus).

On the other hand, Bragg reflection due to the interaction of a neutron wave with a lattice of nuclei has been used to trap neutrons between two single crystal plates of Si[5]. Also, a shift of effective mass of neutrons with energies near the Bragg condition in a crystal was shown[6] by an experiment of neutron propagation through the crystal under diffraction condition. Recently, artificial periodic structures[7,8] of a potential of cold neutrons have been used in neutron physics to investigate the quantum precession and the splitting of neutron spin, tunneling time of a potential barrier and trapping time in potential well in addition to the traditional diffraction and reflection just similar to those for the electron.

Furthermore, a change of decay behavior of neutrons in a strong electromagnetic field was predicted by a calculation[9]. There is a new field of research in the decay behavior of neutrons interacting with other nuclei through electromagnetic and strong interactions.

This paper gives a simple treatment of band structure of low energy (thermal) neutrons in a crystal (neutron band) and a possible trapping mechanism of neutrons related with reflection at a boundary due to a difference of band structures in neighboring crystals. A numerical result is shown by a simple one-dimensional Kronig-Penily model with Fermi quasi-potential, i.e. a delta-function type potential. Possible physics of the system composed of a crystal and the trapped thermal neutron is discussed.

2. Neutron Band

A thermal neutron with a de Broglie wave length comparable with the lattice constant of a crystal behaves as a wave and interacts with nuclei in the lattice (lattice nuclei) through the nuclear force. The interaction could be treated approximately by Fermi pseudo-potential (zero-radius potential[10])

$$V(r)=\frac{2\pi h^2 b}{m}\frac{\delta(r)}{r^2} \qquad (1)$$

with b a parameter with dimension of length (an effective scattering length). The wave function of the neutron with mass m will be calculated with Wigner-Seitz method[11] solving an equation: (2)

$$\{-\frac{h^2}{2mr^2}\frac{d}{dr}(r^2\frac{d}{dr})+V(r)\}\psi(r)=E\psi(r)$$

subject to a boundary condition

$$\left(\frac{\vartheta\psi}{\vartheta r}\right)=0, \quad (\text{at } r=r_0) \qquad (3)$$

where r_0 is the radius of the so-called s-sphere, having the same volume as the atomic volume of the crystal.

To illustrate the essential point of this treatment, we calculate the energy band structure of a particle with mass m in the one dimensional Kronig-Penny lattice with a lattice constant a and an attractive delta-function potential: (4)

$$V(x)=-\frac{h^2P}{ma}\delta(x+na),\ (n=0,\pm1,\pm2,\cdot\cdot)$$

where P is a constant proportional to the intensity of the attractive potential (width x depth). The energy E of the neutron with wave vector k in this crystal is determined by an equational)

$$-P\frac{\sin\alpha a}{\alpha a}+\cos\alpha a=\cos ka \qquad (5)$$

where $\alpha = (2mE/h^2)^{1/2}$. Band structure of this energy spectrum was calculated numerically and plotted in Fig. 1 in the reduced zone scheme ($-\pi \le ka \le \pi$). The value of P was assumed arbitrarily as $3\pi/2$ which corresponds to a square well potential with a depth 2 x 10^3 eV and a width 10^{-13} cm, considering the interaction through the nuclear force. An increase of the parameter P makes the width of the allowed band narrower. The energy of the edge of the lowest energy band is inversely proportional to the square of the lattice constant a^2 and is 2.04 x 10^{-2} eV for $a = 10^{-8}$ cm. It is interesting to note that the energy of this band edge is somewhat lower than the thermal energy at room temperature (300 K) for a lattice with a lattice constant 2 ~ 3 Å.

On the other hand, the wave function of the neutrons in the band has a large amplitude at lattice points where the centers of the attractive potential are. So, neutrons in a crystal have a band structure in their energy spectrum and localized probability amplitude at nuclei at the lattice points.

The neutron band illustrated in Fig. 1 will contribute to trapping of thermal neutrons in a crystal if the crystal is sur-

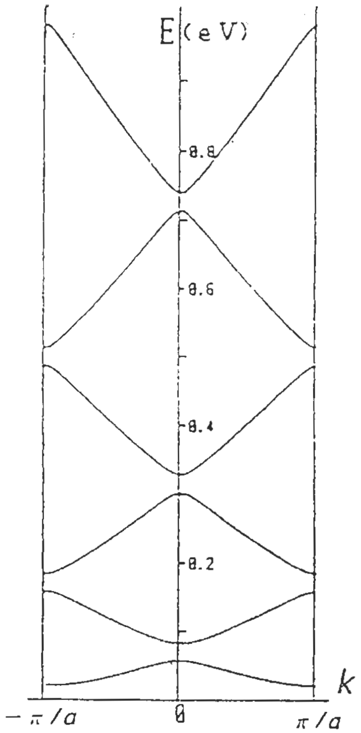

Fig. 1. Energy band structure of neutron in one dimensional attractive delta-function type Kronig-Penny potential. Parameter P is taken arbitrarily as $3\pi/2$ and the wave number is reduced to $|ka| \leq \pi$. For $a = 10^{-8}$ cm, the energy of the edge of the lowest band is 2×10^{-2} eV.

rounded by a wall with a different band structure. A neutron in the crystal can not stay in the wall if the energy of the neutron corresponds to a forbidden energy of the band in the wall. Then, in such a situation, a neutron with a thermal or epi-thermal energy can exist trapped in the lowest neutron band in the crystal if the width of the wall is thick enough to prevent tunneling.

The neutron band in a three-dimensional lattice could be calculated solving Eq. (2) with the potential Eq. (1) and the boundary condition Eq. (3) and is a future program though the essential feature of the neutron band is illustrated above for the one dimensional case.

As the position and width of the allowed band depends on the lattice constant a and the parameter P (proportional to strength of potential), a neutron in a band in one region could be reflected at the boundary of the adjacent region with different lattice constant and/or constituent nuclei. This situation occurs, for instance, in palladium hydrides (deuterides) with a periodic distribution of occluded hydrogen (deuteron) or with a surface layer of alkali (Li) metal on the surface.

The Kronig-Penny model of a potential on the cold neutron has been formed axtificially with a laminar structure of metals[7,8] and the artificial periodic potential thus formed has been used to diffract and reflect neutrons for investigation in neutron physics. In this case, however, the potential is not that given in Eq. (1), but one averaged over nuclei in a layer of the structure to form a diffractive index for the neutron.

3. Discussion

The notion of a neutron band in solids proposed in this paper for the first time is a novel one, corresponding to the popular electron band in solids and the photon band in artificial periodic structures. It is interesting to note that these all the particles are already used in structural analysis as electron, X-ray and neutron diffractions, widely and complementally in science and technology.

On the other hand, those band structures in the energy spectra have fairly different characters. The electron band, as we know well, had been worked out in 1930's and it successfully explained the characteristics of solids and had been the basis of the modern technology. The photon band, using artificial materials with an appropriate period for the wave length of a relevant photon, has recently been recognized.

The electron and photon are stable elementary particles and their properties have been thoroughly investigated. The neutron, in contrast to them, is unstable in its free state, with a decay time of 887.4 ± 0.7 s. Although the interaction of a neutron with solids has been investigated in relation to the structural analysis of matter as the neutron diffraction and with an atomic pile as neutron optics, the state of neutrons in solids has been left almost untouched so far, due perhaps to its unstable nature.

Recently, multi-layer structures of crystals, for instance Permalloy(100Å)/Ge(800Å)/Permalloy(100Å), have been used to investigate trapping and tunneling of a cold neutron[8]. This is a new direction of low energy neutron physics, where the property of a neutron in a potential as an object of research instead of the external effect of a crystal or a potential structure on the neutron investigated hitherto[1-7].

The neutron band investigated in this paper is on the same line of investigation where the artificial potential structure was used for cold neutrons[8], but the difference may be in the interaction of the neutron and the lattice. In the former, the interaction is a strong interaction between the neutron and individual nucleus and in the latter, that through diffractive index of a layer (nuclear force averaged over a layer) due to the difference of wave lengths of the neutrons in the two cases.

There are several possibilities for finding out characteristics of the energy band of thermal neutrons due to the nuclear interaction not found in electron and photon bands due to electrostatic and electromagnetic interactions, respectively. The characteristics of the cold neutrons in the multi-layer films are rather similar to the electron and phonon band and those of the band structure investigated in this paper will be different from them.

The difference is based on the nature of the interaction and will be pointed out as follows: The first is related with the instability of free neutrons for beta decay. The band state is coherent with the lattice structure in its nature and the nuclear interaction of a neutron in it with lattice nuclei may result in stabilization of the neutron against the beta decay. The second is related with interaction of lattice nuclei with a neutron Bloch wave in a band. If there is a nucleus which is unstable for a decay (alpha-, beta-, or gamma-decay), the interaction may influence the time constant of the decay, probably to shorten it. The third is related with interaction of the neutron in a band with a foreign nucleus in the lattice. The foreign nucleus will disturb the neutron Bloch wave and may result in a nuclear reaction (fusion or scattering) of the neutron by the nucleus. These effects might be detected experimentally as novel nuclear events occurring in materials with appropriate structure.

One of characteristics of the neutron band, if we look into details, calculated by the Kronig-Penny model and given in Fig. 1, is the shape of the lowest band. The energy minimum of this neutron band is at $k = \pi/a$ in contrast to at $k = 0$ in the case of the electron band.

This characteristic shape of the lowest band of neutron energy spectrum results in the existence of trapped neutrons with opposite momenta and spins, even when the concentration of the trapped neutrons is very low.

If two trapped neutrons with opposite lattice momenta and spins form a Cooper pair (neutron Cooper pair) by the interaction through phonons, the energy of the system becomes lower to make the life time of the neutron elongated further.

The interaction of a neutron with a nucleus through inhomogeneity of potential in a lattice destabilizes the trapped neutrons for nuclear reactions. In such a case, several nuclear reactions could be expected and as is shown in the previous paper[12], nuclei in a crystal can emit and absorb a neutron without recoil (the neutron Moessbauer effect). The neutron thus emitted from one of nuclei in a crystal can be absorbed by another nucleus without recoil, which in turn can emit a neutron again keeping the neutron in the crystal without limitation of its life time.

The behavior of thermal neutrons in quiet solids have not attracted attention except those works on the external effects of crystals for the neutron cited above[3~8], though there are interesting features of solid state-nuclear physics pointed out above as 1) elongation of neutron life time, 2) destabilization of foreign nuclei in a lattice, and 3) neutron fusion with or scattering by a nucleus exerting a large perturbation on it, which may be more or less interesting than those in high energy neutron physics developed in relation with nuclear reactors.

The author would like to express his thanks to members of his laboratory who have cooperated in research of low energy neutrons in solids, a part of which has been treated in this paper. He is also grateful to Dr. T. Ebisawa of Kyoto University for his kindness in sending him papers from his group on the physics of cold neutrons with artificial potential structure formed by multilayer crystal films.

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