Neutron Scattering
Probing lattice dynamics and magnetic structure

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(Dated: November 24, 2017)

I. MOTIVATION

As humans, we like to "see" matter at atomic length scales in order to better understand how things work. The theory of scattering is a tool to construct a material's structure based on how other matter or radiation bounces or *scatters* off it. Among these probes, neutrons hold a special place: owing to the fact that they have zero charge, neutrons do not interact with atoms via electric forces and can penetrate to large depths in most materials, as compared to X-rays, for example. In addition, because neutrons have a magnetic moment, they interact with the unpaired electrons in magnetic atoms. This can give us valuable information, for instance, about the arrangement and density distribution of these electrons.

In the following sections, we introduce the fundamental ideas that govern scattering and see how they are applied to the experimental study of condensed matter systems.

II. NUCLEAR SCATTERING: CRYSTAL STRUCTURE

In scattering, as with any physical process, the energy and momentum of both the nuclei and neutron are altered individually, but are conserved. Based on the momentum conservation, we define the momentum transfer, by $\hbar\mathbf{q} = \hbar(\mathbf{k}' - \mathbf{k})$ where, $\mathbf{q}$ is called the scattering vector while $\mathbf{k}$ and $\mathbf{k}'$ the initial and final wave vectors respectively. An elastic process is easily distinguished from an inelastic one because the energy of the neutron is unchanged in former case.[1]

Generally speaking, the double differential cross section that describes the scattering process has the form

$$\frac{d^2\sigma}{d\Omega dE'} = \underbrace{\frac{k'}{k}\left(\frac{m}{2\pi\hbar^2}\right)^2}_{\substack{\text{kinematic}\\ \text{part}}} \underbrace{|\langle \mathbf{k}'\sigma'|V|\mathbf{k}\sigma\rangle|^2}_{\substack{\text{interaction}\\ \text{matrix element}}} \underbrace{\delta(E - E' + \hbar\omega)}_{\substack{\text{energy}\\ \text{conservation}}} \tag{1}$$

One of the corner stones in the theory of neutron scattering is Fermi's crucial observation that the neutron-nucleus interaction can be replaced by a pseudo-potential that results in the same scattering while being probed perturbatively via the Born approximation. In a crystal, for ions located at $\mathbf{r}_j$, this is given by [5]

$$V(\mathbf{r}) = \frac{\pi\hbar^2}{m}\sum_j b_j \delta(\mathbf{r} - \mathbf{r}_j) \tag{2}$$

where m is neutron mass and b_js correspond to the scattering lengths and are a measure of the interaction strength between the neutron and the jth nucleus.

Following this insight, Van Hove showed that the scattering law can be written in terms of the time dependent correlations between positions of pairs of atoms in the sample. This, in other words, is the Fourier transform of the probability distribution for finding two atoms separated by some distance [14]:

$$\frac{d^2\sigma}{d\Omega dE'} = \frac{1}{2\pi\hbar}\frac{k'}{k}\int_{-\infty}^{\infty} dt e^{i(E'-E)t/\hbar} \sum_{i,j} b_i b_j \left\langle e^{-i\mathbf{q}\cdot\mathbf{r_i}(0)} e^{-i\mathbf{q}\cdot\mathbf{r_j}(t)}\right\rangle \tag{3}$$

which relates the nucleus i at time zero with nucleus j at time t. This is Van Hove's general result for a typical neutron scattering experiment. This is usually simplified further by averaging over the scattering lengths, which can be justified based on the fact that the spin of a nucleus and its position in space are not correlated. This gives us the expression [14]

$$\sum_{i,j}\langle b_i b_j\rangle A_{ij} = \sum_{i,j}\langle b\rangle^2 A_{ij} + \sum_i \left(\langle b^2\rangle - \langle b\rangle^2\right) A_{ii} \tag{4}$$

where A_{ij} is the expectation value in Eq. 3 and b is the average scattering length of all the nuclei in the system. The assumption that there are no correlations between the b_is of different nuclei lead us to the above relation.

Plugging this into Eq. 3, the differential cross section emerges as a sum of two components, each coming from one of the terms in Eq. 4.

The first one depends on the correlations between different nuclei at different times and gives rise to interference effects. In other words, it corresponds to *coherent* scattering, wherein neutrons scattered from the ions interfere. As this depends on the distances between atoms (via the integral A_{ij}), it encodes information about the structure of the sample. While elastic coherent scattering speaks of the equilibrium structure, the inelastic counterpart probes the collective motions (phonons). This aspect is further discussed in Sec. V.

[1] Throughout the following discussion, we work with the assumption that the neutron energy is too small to change the internal structure of the nucleus. Also, note that the unprimed and primed quantities correspond to initial and final neutron states, respectively.

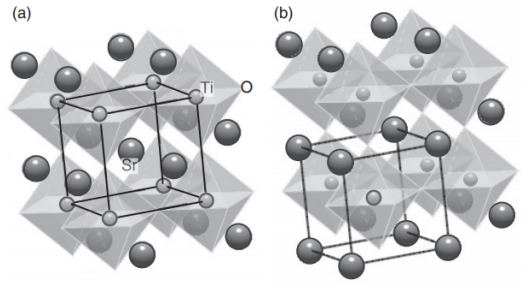

FIG. 1. The idealized perovskite structure of $SrTiO_3$. The solid lines outline the primitive cubic unit cell [5].

The second term, on the other hand, depends only on the correlation of a nucleus with itself at different times and does not show interference. This represents *incoherent* scattering. In this case, the elastic incoherent scattering, being same in all directions, appears as noise. The inelastic component, though, provides information about atomic diffusion.

At this stage, it is illustrative to see how neutron scattering is useful in determining the structure of crystalline compounds. A perovskite crystal typically has the composition ABO_3, where A and B are two different cations. An ideal perovskite has a simple cubic structure (see Fig.1). In reality, however, atoms, usually the oxygens, are displaced from the ideal positions under the influence of neighboring cations – this alters the physical properties of the crystal. In addition to the usual X-ray diffraction techniques, neutron scattering is typically employed to structurally characterize these complex oxides because the neutrons are sensitive to the oxygen atoms.

In the specific case of yttrium-doped barium cerates $BaCe_{1-x}Y_xO_{3-\delta}$ (BCY), neutron scattering can give us an idea of how the yittrium doping modifies the crystal structure. We see this for two specific values in Fig. 2. The peaks correspond to different ionic sites in the crystal. Notice that there is a perceptible difference in the number and position of some of these peaks.

After this basic introduction to the theory behind neutron scattering, we shall now briefly describe ways in which the neutrons needed for these experiments are actually generated and handled.

III. NEUTRON SOURCES

There are two ways for providing the neutrons for scattering experiments. They can either be generated through fission in reactors or in accelerator-based spallation sources, i.e. through ejecting particles from a target due to impact. The resulting neutrons of both of these processes have energies of order 1 MeV, but for most scattering experiments only neutrons with energies of 1 eV or less are needed. Therefore special devices called *moderators* are used to slow them down.

In fission reactors, a fissile nucleus, like ^{235}U captures a neutron n and then splits into fission fragments or atoms

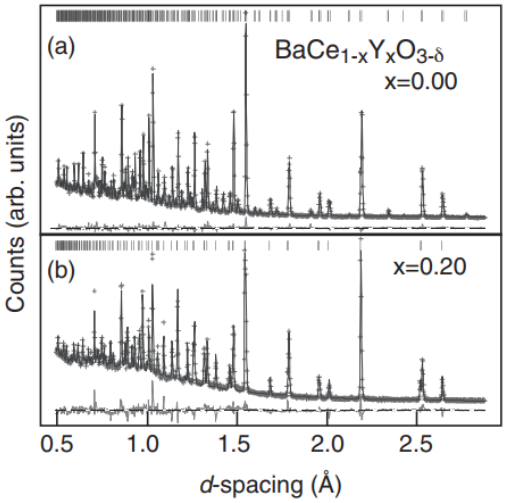

FIG. 2. Observed diffraction intensities for BCY at room temperature, with $\delta = x/2$. A difference curve between observed and calculated intensity is shown below each profile [5].

of smaller atomic weight (X, Y) and in average 2.5 fast neutrons per collision: $^{235}U + n \rightarrow X + Y + 2.5n$. One of these neutrons is needed to self-sustain the fission process, around 0.5 are lost and one neutron can be used externally for the scattering experiment. Both the experiment and the fission reaction require less energy than the generated 1-2 MeV. So, in moderators, the velocity of the neutrons as well as the temperature of the system are reduced by inelastic scattering with light elements, e.g. H_2O or D_2O. Fast neutrons are scattered or reflected back into the moderator material by reflectors being located outside the moderator. The energy distribution as well as the exact distribution of the background consisting e.g. of fast or delayed neutrons and gammas, can be varied by changing the reflector or moderator.

Spallation sources are often pulsed, in order to do time-of-flight measurements of the neutron energy (see Sec. IV C). So, for the acceleration of the particles, which are used to generate the neutrons, a synchrotron or an accumulator is used. The thereby accelerated high-energy particles, usually protons with at least an energy of 1 GeV, impinge on heavy targets. Due to this bombardment, high-energy neutrons, pions and spalled nuclei appear, that themselves collide, generating internuclear cascades, that result in excited nuclei. Nuclei relaxation back to the ground state provides the neutrons, whose spectrum also has an maximum at approximatively 2 MeV. When generating neutrons with spallation sources, they also have to be slowed down by scattering events in moderators. These moderators broaden the pulses, which is especially a big problem for short-pulse spallation sources. So, for ensuring that the pulse is still sharp enough, special geometries and absorbing materials are used. Placing absorbing materials around the moderator in a strategic way prevents slow neutrons from reentering in the moderator and through that from

contributing to the pulse that is used for the experiment [2].

IV. NEUTRON INSTRUMENTATION

Our discussion in previous sections focused on the fundamental idea behind neutron scattering, its domain of applicability and general characteristics of neutrons scattered by periodic arrays of ions, as well as on ways of producing the neutrons for the experiments. In this section we describe the actual experimental devices required to measure various quantities derived earlier. As in any scattering experiment, the measurements revolve around three objects [11]:

- $\sigma_{tot}(E)$, the total cross section as a function of incident neutron energy E (for coherent elastic processes);
- $\frac{d\sigma}{d\Omega}(\mathbf{q})$, the differential cross section for (for incoherent elastic processes);
- $\frac{d^2\sigma}{d\Omega dE'}(\mathbf{q},\omega)$, the phonon energy and momentum dependent double differential cross section (for inelastic processes).

The first two are mostly measured with diffractometers and reflectometers, and the last one with spectrometers. The main difference between the two is that diffractometers do not analyze the outgoing beam, they simply detect the neutrons at a given scattering angle (thus obtaining the total cross section). If scattering is almost purely elastic, that is all that is needed, as energy and momentum of detected neutrons are identical to those of the incoming beam anyway and the only information to be gathered is the scattering angle. Meanwhile spectrometers, dealing with inelastic scattering, have to analyze the outgoing beam for energy dependence, because in general there will be multiple energy and momentum "neutron groups" scattered at a given angle due to interactions with various kinds of phonons.

Both of these types of devices are ultimately made up of the same structural components. We split them into three groups: (a) incident beam manipulation, (b) sample management, and (c) scattered beam measurement.

A. Incident beam manipulation

Control over the incoming neutron beam is key to a successful scattering experiment. From ensuring sufficient resolution, to filtering out thermal neutrons, to monochromatizing the beam, there is no shortage of challenges. Over the years special tools have been developed to address each of these in turn.

Whether one is looking at elastic Bragg diffraction, or inelastic phonon production, it is often the case that a monochromatic beam of neutrons is desired. This is traditionally accomplished by using a crystal with predetermined Bragg scattering peaks of its own, preferably with a small overall absorption cross section. According to the Bragg formula $\lambda = 2d_M \sin\theta_M$, from a mixed initial beam only certain neutrons will scatter efficiently along a given angle θ_M: thus one effectively "filters" the mixed beam. Moreover, adjusting the incidence angle gives one exquisite control over the characteristics of the new beam. Such a device is called, unsurprisingly, a *monochromator*. Typical crystals to be used are pyrolytic graphite, Si, Ge, and best of all, Be [11].

Although a monochromator allows for sharp neutron energy selection, oftentimes the neutrons coming out of the source are simply too fast and do not have the desired energy in their mix to begin with. This is where the moderator, already mentioned in Sec. III, comes in handy, reducing neutron velocity to the desired range.

Even in the simplest neutron scattering setups, like those in regular diffraction experiments, where the only free parameter is the incidence angle, neutron beams have to travel considerable distances between the source and the target[2] and any filters, monochromators, moderators, and other devices in-between. As a consequence, it is very important to main beam alignment and minimize losses. One incredible commonplace device serving this goal is the *collimator*: in its simplest iteration [14] this is a pair of slits of converging width, which reduce the spatial extent of the beam and also serve to narrow its angular spread, making it more unidirectional ("collimated"). As for reducing losses, a *neutron guide* can be constructed out of special materials tuned to totally reflect neutron particles internally below a certain angle of incidence. This effectively confines them to the guide and eliminating the $1/r^2$ intensity loss common to any other beam tube (just like in a regular waveguide familiar from classical electrodynamics).

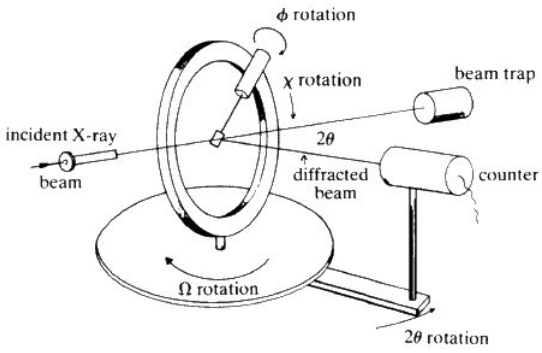

FIG. 3. 4-circle goniometer, to rotate the sample freely about any axis [1].

[2] Typically in order to avoid stray unshielded radiation from the source.

B. Sample management

Typically neutron scattering experiments are conducted on two types of samples: large single crystals, or powders. The two naturally require different kinds of sample holders. For instance, where the experimenter might simply hold the large crystal in place with a holder, in the case of a powder she is forced to use a container of some sort, which is now necessarily in the way of the beam. Usually the container is made out of a material with a very low σ_{el}^{coh}, such as vanadium [11], to avoid introducing additional Bragg peaks. Whereas in a powder the crystalline directions are randomized and thus rotating through a single angle is sufficient to obtain the cross section, a single crystal is usually placed in a *4-circle goniometer* (Fig. 3) to allow for studying as many crystal planes as possible. The 4-circle arrangement allows for rotating the sample freely about any axis. Finally at this stage any additional environment effects may be introduced: be it temperature control (usually a cryostat, to cool the sample below room temperature), an electric or magnetic field, or some other phenomenon whose effect on the sample's crystal and magnetic structure or phonon spectrum is to be studied.

C. Scattered beam measurement

No scattering experiment is complete without the detection of scattered particles and precise measurement of their momenta and energies. In neutron scattering this information is generally obtained one of two ways: inserting an additional Bragg diffracting crystal, exactly like for monochromatizing a beam (in this case the crystal is called the *analyzer*), or using the so-called *time-of-flight* technique. The latter allows one to determine the energy distribution of neutrons at a given scattering angle by looking at their velocity distribution [5]: to figure out their velocity at the time they hit the detector, one needs a pulsed neutron source, instead of a steady one (see sec. III). Given this pulse, a device called a *chopper* can be used to allow only the neutrons with a given range of velocities to pass through. In essence a chopper is simply a time-variable gate that could be opened and closed at will: setting it to open and close sinusoidally selects a given velocity range. Knowing the velocity range, as well as the initial pulse production time and the neutron detection time allows to determine the time of flight and thus that neutron's velocity.

Of course, no beam measurement would be complete without actual particle detection. Typical strategies used for, say, electrons or photons do not work, as neutrons carry no charge and too little kinetic energy. The idea is to use the neutron to initiate some sort of a nuclear reaction that has a charged particle or light as a by-product, then use standard techniques to detect those. A common reaction pathway is with helium, $n +^3 \mathrm{He} \rightarrow^3 \mathrm{H} +^1 \mathrm{H} + 0.7\,\mathrm{MeV}$ [5]: the photon emitted passes through a photo-multiplier until the signal is sufficiently amplified and can be picked up by regular instruments.

Having finished the discussion of general principles of neutron scattering, we move on to demonstrate the utility of the technique on some examples.

V. EXAMPLE A: LATTICE DYNAMICS

One definite advantage of neutrons over other kinds of probes traditionally used in scattering experiments (X-rays, electrons) is that their energies are on the same order as that of phonon modes in most solids [10]. This makes them ideally suited for mapping out the phonon dispersion curves and density of states, which in turn allow the determination (or independent confirmation) of many macroscopic quantities of interest. Some examples include[3]:

1. Speed of sound (slopes of acoustic branches);
2. Elastic constants for use in continuum stress-strain equations (e.g. bulk modulus);
3. The lattice contribution to specific heat (which gives the characteristic T^3 dependence in the intermediate to high temperature regimes);
4. Phonon lifetime (arising from higher-order corrections to the harmonic approximation [6], that is, from phonon-phonon scattering);
5. Thermal transport properties;
6. Debye frequency ω_D, which is relevant for the BCS formula $k_B T_c = 1.13\hbar\omega_D e^{-\frac{1}{N(\mu)V}}$.

Theoretically, phonon dispersion relations can be calculated in the harmonic approximation using standard methods of second quantization, i.e. by writing the ionic displacements in terms of creation/annihilation operators, and only basic knowledge of crystal structure is required. Solutions may always be found analytically, as only two-operator terms are kept in the lattice Hamiltonian. However, this requires the knowledge of force constants $\partial^2 V(\mathbf{r}_i - \mathbf{r}_j)/\partial\mathbf{r}_i\partial\mathbf{r}_j$ of the inter-ionic potential. If we had a way of obtaining the phonon dispersion experimentally, we could determine the force constants by a fit to the experimental results [8], thus constraining the free parameters of our theoretical model. The model can then subsequently be used for further calculations

[3] Note that while most of these require the knowledge of the phonon dispersion (which necessitates, as remarked earlier, the use of a relatively large single crystal), the density of states (which can be calculated accurately even in the presence of many non-aligned crystals and defects) will be able to supply some of that information [7].

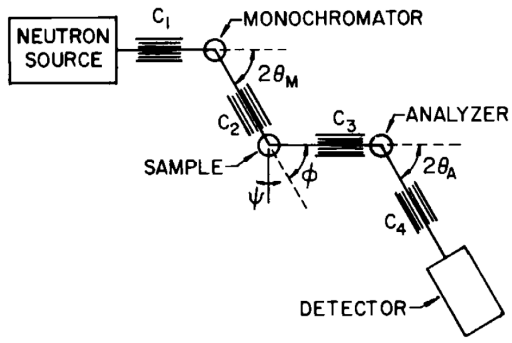

FIG. 4. A diagram of a triple-axis spectrometer [11].

(transport, electron-phonon coupling, etc.). This (and the list above) is certainly ample justification for finding a way to measure phonon dispersion.

A brilliant methodology for experimentally measuring phonon dispersion, due to B.N. Brockhouse [3], has blown the field of inelastic neutron scattering wide open and

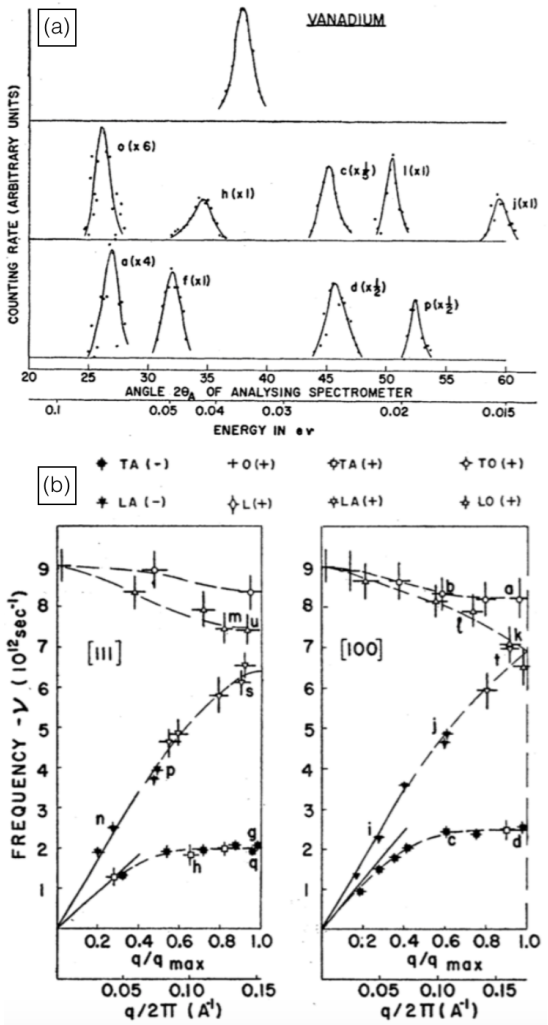

FIG. 5. (a) Neutron energy groups. (b) Corresponding locations on the phonon dispersion curve [4].

even earned him a Nobel prize in 1994. It involves a device known as a *triple-axis spectrometer* [14] — see Fig. 4. Given a beam of neutrons (exiting a nuclear reactor via a small opening), make it monochromatic by passing it through a monochromator (first axis), as seen in fig. 1: this gives one control over $\mathbf{k}, E$ of the incident beam. The now monochromatic beam then hits the sample at some other angle ψ (second axis): this allows to study various orientations of the crystal relative to the incident beam, similar to the rotating crystal technique. Finally, the scattered neutrons $\mathbf{k}', E'$ exiting at all possible angles ϕ are passed through analyzer (third axis) to study the distribution of neutrons with energy at a given angle ϕ.

As neutrons are scattered by the sample, they interact differently with the various phonon branches (assuming the crystal orientation is such that the branches are non-degenerate), thus exiting with different energies along the same scattering angle ϕ. As a consequence we expect to see a number of different "neutron energy groups" at the same angle ϕ, based on which phonons they generated whilst in the sample: these will correspond to peaks (Fig. 5) in the count-energy spectrum produced by the analyzer. In general there will be both elastic and inelastic, coherent and incoherent scattering (see Sec. II). The elastic contribution to this cross section obeys $\mathbf{k} = \mathbf{k}'$, $E = E'$ and thus can be readily eliminated from the count-energy spectrum (simply subtract off the neutrons with identical energy E' identical to the original beam energy E at every angle ϕ). Assuming the incoherent contribution to the differential cross-section is small[4] compared to the coherent one (which is the case for a good number of systems [14], but not all [9]), one may use the inelastic conservation equations

$$\frac{\hbar^2}{2m}(k^2 - k'^2) = \hbar\omega_{\mathbf{q}s}, \quad \mathbf{k}' - \mathbf{k} = \mathbf{q} - \mathbf{G}, \tag{5}$$

on the peaks in the count-energy spectrum to backtrack and determine the phonon energy and wavevector. The peaks are discrete, because only select neutrons $\mathbf{k}'$ satisfy both conservation conditions above. Finally, by changing the angles θ_M and ϕ one can obtain the entire spectrum in this way: the match between theory and experiment obtained in this way is often rather spectacular (Fig. 5). The triple-axis spectrometer technique thus provides a handle on phonon dispersions, allowing to fix free parameters in theoretical models and to independently determine a variety of material characteristics from the spectra.

[4] In the opposite regime, one measures the phonon density of states instead, which gives similar information. Intermediate cases are more difficult to resolve [3].

VI. EXAMPLE B: MAGNETIC SCATTERING

As mentioned earlier, neutron's magnetic moment $\boldsymbol{\mu}_\mathrm{n}$ is used to probe the magnetic structure of matter, through their interactions with the unpaired electrons. While elastic neutron scattering is used to determine the magnetic structure and the density distribution of the unpaired electrons, inelastic scattering gives information about magnetic excitations.

Eq. (1) shows, that the cross section depends on the scattering potential. In the case of magnetic neutron scattering, this is the magnetic potential

$$V_\mathrm{M}(\mathbf{r}) = -\boldsymbol{\mu}_\mathrm{n}\mathbf{B}(\mathbf{r}), \tag{6}$$

which arises from the magnetic moment $\boldsymbol{\mu}_\mathrm{n} = -\gamma\mu_\mathrm{N}\boldsymbol{\sigma}$ of the neutron and the magnetic field $\mathbf{B}$ created by an electron. $\mu_\mathrm{N} = -\gamma\frac{e\hbar}{2m_\mathrm{p}}$ is the nuclear magneton, m_p is the mass of the proton, γ is a constant ($\gamma = 1.913$) and $\boldsymbol{\sigma}$ is the Pauli spin operator for the neutron. $\mathbf{B}$ is a superposition of a magnetic field originating from the spin of the electron and one due to its orbital motion. Evaluating the resulting matrix element, for example, for elastic scattering from magnetically ordered crystals, gives the elastic cross section

$$\left(\frac{d\sigma}{d\Omega}\right)_\mathrm{el} = (\gamma r_0)^2 N \left\{\frac{1}{2}gF(\boldsymbol{q})\right\}^2 \mathrm{e}^{-2W} \sum_{\alpha\beta}(\delta_{\alpha\beta} - \hat{q}_\alpha\hat{q}_\beta) \times \sum_l \mathrm{e}^{i\boldsymbol{q}\cdot\boldsymbol{l}}\langle S_0^\alpha\rangle\langle S_l^\beta\rangle. \tag{7}$$

Here, $(\gamma r_0)^2$ is the magnetic scattering length, which is the magnetic counterpart to the scattering length b we saw in Sec. II: the two are of similar magnitude. $F(\boldsymbol{q})$ is the magnetic form factor, which gives the spatial extend of the spin density around the atoms. g is the Landé-factor. The Debye-Waller factor e^{-2W} is a measure of thermal lattice vibrations and, therefore, describes the temperature dependence of the intensity of the elastically scattered radiation at a crystal. The second sum is the Fourier transformation of the spin pair correlation function, where l labels the site in the lattice and α and β label x, y, or z [14].

One of the most famous examples of magnetic neutron scattering is a measurement of C. G. Shull, who won the Nobel prize together with B. N. Brockhouse. He analyzed the structure of MnO-crystals, which led to the confirmation of antiferromagnetism [12, 13]. MnO has a conventional cubic structure. The neutron diffraction pattern at room temperature (see Fig. 6(a), bottom), as expected, shows the regular Debye-Scherrer diffraction peaks for a cubic crystalline structure at both, all-even and all-odd lattice sites. However, when lowering the temperature below the Néel-temperature of MnO, the nuclear scattering peaks remain, as shown in Fig. 6(a) (top), but there also appear additional magnetic scattering peaks at new positions. For explaining these, one cannot use the conventional chemical unit cell of MnO. Instead, as now the pattern only shows all-odd peaks ((111), (311), (331), (511)) the new, magnetic unit cell must be doubled in comparison to the chemical one, which indicates that MnO has two sublattices with opposite electron spins (Fig. 6(b)). Thus, the interaction of the magnetic moments of the scattered neutrons and the valence electrons of the crystal clearly shows the antiferromagnetic structure of MnO.

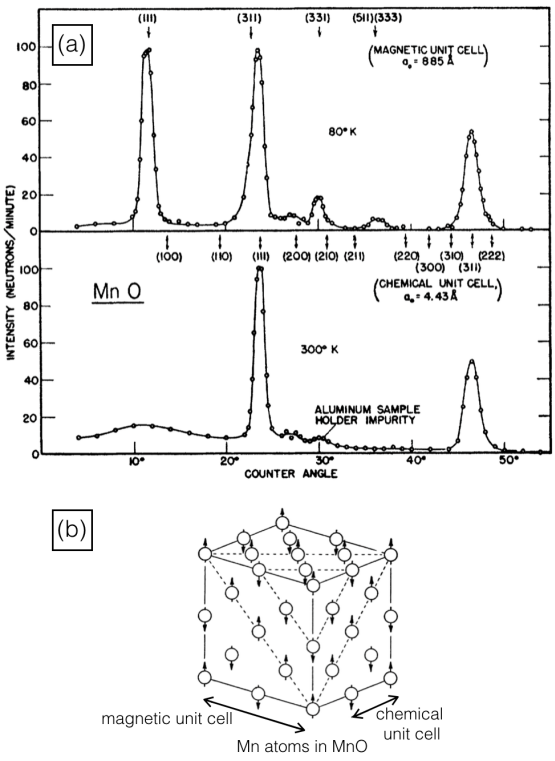

FIG. 6. (a) Neutron diffraction patterns for MnO at 80 K and at 300 K. At low temperature, four extra diffraction peaks appear. (b) Chemical and magnetic unit cell of MnO [12].

VII. CONCLUSION

Charge neutrality and strong magnetic moment make neutrons very suitable for use in scattering experiments that probe structures on the scale of interatomic distances. Neutrons penetrate deep into the bulk of the material, allowing to image the crystal structure more fully, to investigate phonon modes, as well as magnetic structures or excitations. Depending on the imaging technique of choice – say, time-of-flight method or the triple-axis spectrometer – different neutron sources can be chosen to accommodate the needs of the apparatus, be it the nuclear reactor produced steady beam or the pulsed beam of spallation sources. Neutron scattering, described theoretically by the differential cross section, is thus a powerful technique, that together with other experimental methods like electron microscopy and nuclear magnetic resonance to better characterize the properties of matter.

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