Physics of Debye-Waller Factors

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Abstract

This note has no new results and is therefore not intended to be submitted to a ”research” journal in the foreseeable future, but to be available to the numerous individuals who are interested in this issue. The Debye-Waller factor is the ratio of the coherent scattering or absorption cross section of a photon or electron by particles bound in a complex system to the value for the same process on an analogous free particle. It is often interpreted also as the probability of the coherent process, normalized to unity, with the difference between unity and the Debye-Waller factor interpreted as the probability of incoherent processes. The Debye-Waller factor is then interpreted as a measure of decoherence. The breakdown of this description for a test particle which cannot give or lose energy is not generally appreciated. Prime examples are: Bragg scattering, the Mössbauer effect and related phenomena at zero temperature. The physics of the change in the interpretation of the Debye-Waller factor is summarized here in a hopefully pedagogical manner.

I. INTRODUCTION

When a particle is scattered by another particle which is bound in a complex system, the probability of elastic scattering with no change in the state of the complex system is proportional to a quantity called the Debye-Waller factor. This originally arose in the scattering of X-rays by atoms in a crystal, where the probability of coherent scattering was proportional to the Debye-Waller factor, which was always less than unity, and depended upon the temperature of the crystal. There was also a probability of incoherent scattering. The sum of the squares of the incoherent and coherent scattering amplitudes from a given
atom was always equal to the square of the scattering amplitude from a free atom. The Debye-Waller factor might be interpreted as a measure of decoherence. However, this is not generally true, and the physics of decoherence and dephasing in processes where a test particle cannot gain or lose energy has been discussed in detail [1]. We focus here on the probability interpretation and the relation between analogous processes on free vs. bound particles.

In any process described by the Golden Rule of time-dependent perturbation theory that involves a final state with at least one particle in a continuum the transition probability per unit time is proportional to the product of the square of the transition matrix element and the density of allowed final states. In X-ray scattering by crystals and in Mössbauer transitions the energy of the outgoing X-ray is so large compared to lattice excitation energies that the difference in phase space over the entire elastic and inelastic spectrum can be negligible. In other cases it may not be negligible. In all cases the square of the transition matrix for coherent elastic scattering is reduced by the Debye-Waller factor from the square of the matrix element for scattering from a free particle. But this reduction is not a result of decoherence.

This can be seen by simply writing the expression for the transition matrix element between a given initial state $|i\rangle$ of the complex system and a given final state $|f\rangle$ for the scattering of an incident particle by a component of the complex system whose co-ordinate is $\vec{x}$

$$\langle f| T |i\rangle = g(\vec{k}) \langle f| e^{i\vec{k} \cdot \vec{x}} |i\rangle$$  \hspace{1cm} (1.1)

where $\vec{k}$ is the momentum transfer and $g(\vec{k})$ is the strength of the interaction causing the scattering.

This expression clearly satisfies the sum rule,

$$\sum_f |\langle f| T |i\rangle|^2 = |g(\vec{k})|^2$$  \hspace{1cm} (1.2)

while the square of the transition matrix for scattering without changing the state of the complex system is given by
\[ |\langle i | T | i \rangle|^2 = |g(\vec{k})|^2 |\langle i | e^{i\vec{k} \cdot \vec{x}} | i \rangle|^2 \] (1.3)

For the case where the initial state is a free particle, there is only a single final state in the sum and the quantity \( |g(\vec{k})|^2 \) is just the square of the transition matrix element for scattering on a free particle. This naturally leads to the description in which the square of the transition matrix element for scattering without changing the state of the complex system is given by the product of the quantity \( |g(\vec{k})|^2 \) and the Debye-Waller factor \( |\langle i | e^{i\vec{k} \cdot \vec{x}} | i \rangle|^2 \). For cases where the transition probability is proportional to the square of the transition matrix element with the same proportionality factor for all final states \( |f\rangle \) the Debye-Waller factor gives the relative probability of elastic scattering vs. inelastic scattering, where the total probability of elastic and inelastic scattering is normalized to unity.

\[ \sum_f |\langle f | e^{i\vec{k} \cdot \vec{x}} | i \rangle|^2 = 1 \] (1.4)

This picture of the Debye-Waller factor as defining a relative probability of coherent vs. incoherent scattering, or of elastic vs. inelastic processes has entered the folklore in many areas of physics, but it is not strictly correct. It is an approximation which holds only in a certain kinematic region.

A problem arises because the transition probability is not simply proportional to the square of the transition matrix element. There is also an additional kinematic phase space factor. In the case of X-ray scattering by crystals and the Mössbauer effect, the change in the phase space factor over the elastic and inelastic spectra is negligible and one can accept the probability interpretation. When the available phase space for the final state is not a constant over the entire spectrum, the expression for the elastic transition, (1.3) is still valid, but the Debye-Waller factor can no longer be interpreted as a probability. It represents the reduction factor for the elastic transition from a bound system relative to that for the scattering from a free particle, but the sum of the elastic and inelastic transitions no longer satisfies the sum rule (1.2) and there is no longer a normalized probability.

Consider, for example, the scattering of a photon by an Einstein crystal in its ground state; i.e. at zero temperature. If the energy of the photon is less than the energy required
to excite one phonon, there can only be elastic scattering. The transition matrix elements for transitions to all states of the lattice are still given by eq. (1.1), and the cross section for elastic scattering by an atom in the lattice is still reduced by the Debye-Waller factor from the value of the cross section for elastic scattering by a free atom. But there is no inelastic scattering and the total scattering cross section is reduced from the free atom value. The sum rule (1.2) relates transition matrix elements but not probabilities.

If the scattering is observed at a Bragg angle, the coherence of the amplitudes scattered from different atoms in the crystal gives the normal Bragg peak in the angular distribution with an intensity for coherent scattering proportional as usual to the Debye-Waller factor. But here there is no incoherent scattering. All the scattering is coherent. The Debye-Waller factor does not produce decoherence. At a finite temperature where there is a possibility that the photon can gain energy in the scattering process, this inelastic scattering is incoherent. But the variation with temperature of the coherent scattering is described by the Debye-Waller factor independently of the additional incoherent inelastic scattering. The Debye=Waller factor does not produce incoherence nor decoherence.

When this is applied to the scattering of an electron at the top of a Fermi sea at zero temperature by either an electron gas in a metal or by impurities, each individual scattering is reduced by its individual Debye-Waller factor. But there is no inelastic scattering because the electron can neither gain nor lose energy. It cannot gain energy from the rest of the system at zero temperature and it cannot lose energy since it is at the top of a Fermi sea. The total scattering cross section is reduced. At each interaction the probability that the electron escapes without scattering is increased above the normal probability for the case where it has the same energy and the Fermi sea is unoccupied. Thus mean free paths become larger and other effects normally ignored become more important.
II. DEBYE-WALLER FACTORS FOR MACROSCOPIC SYSTEMS

In a completely different context we note that the Debye-Waller factor plays an interesting role in interference experiments with photons scattered by mirrors. One may be tempted to consider the mirrors as classical objects, and use classical kinematics to describe the momentum and energy transfer to the mirror when the photon is scattered. Since this momentum and energy is tiny, one can envision a very sensitive device which can use this tiny energy as a trigger (e.g. by exploding a bomb) to give evidence of the scattering of the photon by this particular mirror and destroy the interference. Conversely, if the photon is detected without exploding the bomb this can be evidence that the photon was scattered by another mirror that was not coupled to the bomb.

The fallacy in such arguments is that the mirrors themselves are subject to the laws of quantum mechanics. Since they must be bound to a fixed position in space, they will be described by quantum states with a discrete energy spectrum. The allowed values of energy transfer to the mirror when the photon is scattered must correspond to the energy differences between energy levels of the bound mirror. The scattering of a photon by a mirror will therefore be either elastic, in which case the mirror remains in the same initial energy level and there is no energy transfer to the mirror, or it will be inelastic, in which case the mirror jumps to a different energy level.

The tiny energy transfer given by the classical result for the scattering of a photon by a mirror can be interpreted by the correspondence principle as only the average energy transfer. In all practical cases this tiny energy transfer is very much smaller than the energy level spacings. Thus the probability of elastic scattering in which there is no energy transfer and therefore no probability of triggering a bomb will be very close to unity. It is given by the Debye-Waller factor $|\langle i | e^{i\vec{k} \cdot \vec{x}} | i \rangle|^2 \approx e^{-k^2<x^2>}$ where here $|i\rangle$ denotes the initial quantum state of the mirror, $k$ is the momentum transfer and $<x^2>$ is the mean square fluctuation in the position of the mirror. Since the position fluctuation must be tiny in comparison with the wave length of the photon in any realistic experiment, the Debye-Waller factor will be
very close to unity, and the probability that sufficient energy is transferred to the mirror to trigger a bomb is vanishingly small.

Another way to describe the same physics is to note that the kinetic energy transfer to the mirror by the recoil momentum of scattering a photon is not only tiny compared with the spacing between the energy levels of the bound states of the mirror, but also tiny in comparison with the zero-point kinetic energy of the mirror in its bound state. Since the only allowed energy transfer is the energy difference between energy levels, the probability that a tiny change in kinetic energy can produce a quantum jump to another energy level is negligible.

Another context with similar physics is in the detection of neutrinos in a neutrino oscillation experiment. Neutrino oscillations arise because the neutrino state incident on the neutrino detector is a well-defined coherent mixture of states having different masses, different momenta and different energies. Particle physicists tend to overlook the fact that the neutrino detector is a quantum-mechanical condensed matter system and that the neutrino detection process involves a Debye-Waller factor. Coherence is preserved between incident neutrino states having the same energy, different masses and different momenta because the Debye-Waller factor is very close to unity and the transition from these different mass eigenstates lead to the same final state of the detector. However, incident neutrinos with different energies produce final states of the detector with different energies and all phase information between neutrino states with different energy is lost. This causes confusion among particle physicists who are accustomed to treat energy and momentum as different components of the same four-vector and cannot understand why states with the same energy should be coherent and states with the same momentum and different energies are not. But the interaction with the detector breaks the energy-momentum symmetry. The detector is a condensed matter system initially in thermal equilibrium and described in its rest system by a density matrix which is diagonal in energy but not in momentum.
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