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Coherent pair production by energetic gamma rays incident on quasicrystals

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Abstract

We develop a Born-approximation theory of coherent pair production (CPP) of electrons by energetic gamma rays incident on an icosahedral quasicrystal, described by a schematic model (K model) that includes phonon and phason disorder. Our main result is a formula for the cross-section $d\sigma_{cpp}/d\varepsilon_+$ for CPP, differential with respect to the positron energy ε_+ and of order α^2 in the fine-structure constant $\alpha \approx 1/137$, but which is otherwise exact. We discuss results of numerical calculations of $d\sigma_{cpp}/d\varepsilon_+$ versus $y = \varepsilon_+/k$ for gamma rays of energies $k = 20$ MeV, 200 MeV, and 3 GeV, incident on icosahedral Al–Mn–Si, described as a special case of the K model (vertex model). This consists in placing an Mn atom at each vertex of the relevant Ammann tiles. Our calculations include CPP of types A and B. Both types exhibit vertical intensity drops at irregularly distributed y-values, many of these drops being so large that they should be observable experimentally. They are analogous to the large intensity drops exhibited by coherent bremsstrahlung in quasicrystals. We predict that CPP drops also occur for realistic models of i-Al–Mn–Si at the same y-values as for the vertex model, but whose magnitudes may differ from those predicted by this model.

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1. Introduction

Coherent bremsstrahlung (CB) and coherent pair production (CPP) in crystals have been extensively investigated, both experimentally and theoretically (see, e.g. [1–3] and the references cited therein). This is not the case for CB in quasicrystals (QCs), about which to our best knowledge only two papers, one theoretical [4] and the other experimental [5] have been published.

The present paper initiates the theoretical investigation of CPP in a class of icosahedral quasicrystals (IQCs) with phonon and phason disorder, which we describe by a simple model (K model) (for a thorough discussion of phasons in IQCs, see [6]). Our main result is a Born-approximation formula for the cross section, differential with respect to the electron (or positron) energy, for CPP production in such IQCs. It is derived by an exact integration of the contribution of the two lowest order Feynman diagrams involved (Fig. 6). Using this formula, we compute this cross section numerically for 20 MeV, 200 MeV, and 3 GeV photons incident on icosahedral Al–Mn–Si (i-Al–Mn–Si), described by a specialization of the K model (vertex model) [7]. Our calculations, which deal with CPP of types A and B (defined in Section 3), predict the occurrence of irregularly distributed drops in electron intensity, many of which should be experimentally detectable. We predict that such drops also occur for realistic models of i-Al–Mn–Si at the *same* values of electron energy as for the vertex model, but whose magnitudes may differ from those predicted by this model.

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About 100 intermetallic compounds of icosahedral quasicrystalline structure have been known since the early 1990s [8,9]. Complete structural information is lacking for many of them. The main reason for this is that the quasiperiodicity present in these compounds introduces too many structural variables for X-ray or neutron diffraction analyses to cope with. For this reason, theoretical studies such as those in [4] and the present paper promise to be useful tools for arriving at a better understanding of the structure of real IQCs.

The organization of this paper is as follows. Section 2 consists of two subsections. In Section 2.1 we review some basic quasicrystallographic facts needed to define the K model. Section 2.2 contains a discussion of the relativistic kinematics of CPP in IQCs of the type considered here, together with a statement of the above Born-approximation formula for such production in the K model, whose proof is summarized in Appendix B. This formula was obtained by an exact evaluation of the contributions of the two Feynman diagrams alluded to above (Fig. 6). Certain well-known quasicrystallographic facts stated in Appendix A are also used in its proof. Numerical results obtained using this formula are discussed in Section 3, where special attention is paid to the occurrence of large intensity drops in CPP in IQCs described by the K-model. An analogous Born-approximation formula, also exact, for CPP in crystals of diamond structure is stated in Appendix C, for the sake of completeness. Finally, Appendix D contains mathematical results, which shed light on some of the numerical ones discussed in Section 3.

For the convenience of readers who are primarily interested in the experimental predictions of the theory of CPP production in quasicrystals, rather than in their mathematical proofs, such proofs have been largely relegated to the appendices. The main exception to this rule is the explanation of the intensity drops in CPP production given in Section 2.2 on the basis of simple relativistic kinematics, which to our best knowledge has not been discussed heretofore in the literature.

2. Theory of CPP by high-energy gamma rays incident on a model IQC

2.1. Auxiliary quasicrystallographic facts and definition of the K model

The icosahedral IQCs known at present fall into two classes. Those of the first class can be generated by the well-known projection method [10,11] applied to a six-dimensional simple cubic lattice, while those of the second are obtainable by projecting a six-dimensional body-centered cubic lattice [6]. For reasons of simplicity, the present study will only consider CPP production in IQCs of the first class.

Turning our attention to IQCs of this class, we consider the six-dimensional simple cubic lattice

$$\Lambda = \left\{ a \sum_{i=1}^{6} m_i \varepsilon_i : m_i \in \mathbf{Z}, \quad i = 1, \ldots, 6 \right\}, \tag{1}$$

of side length a, where $\varepsilon_1 = (1,0,0,0,0,0), \ldots, \varepsilon_6 = (0,0,0,0,0,1)$, the standard basis in $\mathbf{R}^6$, and $\mathbf{Z}$ denotes the integers. We define E, E' as the mutually orthogonal, three-dimensional subspaces into which $\mathbf{R}^6$ is mapped by the respective projection operators Π, $\Pi' = I - \Pi$, where I is the unit operator in $\mathbf{R}^6$ and Π has the matrix representation

$$[\Pi_{jk}]_{j,k=1,\ldots,k} = (1/2\sqrt{5}) \begin{bmatrix} \sqrt{5} & 1 & -1 & -1 & 1 & 1 \\ 1 & \sqrt{5} & 1 & -1 & -1 & 1 \\ -1 & 1 & \sqrt{5} & 1 & -1 & 1 \\ -1 & -1 & 1 & \sqrt{5} & 1 & 1 \\ 1 & -1 & -1 & 1 & \sqrt{5} & 1 \\ 1 & 1 & 1 & 1 & 1 & \sqrt{5} \end{bmatrix}, \tag{2}$$

with respect to the above basis. The space E is identified with ordinary physical space, and E' is commonly called *perpendicular space*. If $\mathbf{X} = \Pi\mathbf{Y}$ and $\mathbf{X}' = \Pi'\mathbf{Y}$, where $\mathbf{Y} \in \mathbf{R}^6$, the three-dimensional vectors $\mathbf{X}, \mathbf{X}'$ are said to be a *complementary pair*, or simply to be complementary. If $\mathbf{Y} \in \Lambda$, the vectors of each complementary pair X, X' are in 1-1 correspondence [10].

Let L denote the projection of the hypercubic lattice (1) into E, i.e.

$$L = \Pi\Lambda = \left\{ a \sum_{i=1}^{6} m_i \mathbf{e}_i : m_i \in \mathbf{Z}, \quad i = 1, \ldots, 6 \right\}, \tag{3}$$

where $\mathbf{e}_i := \Pi\varepsilon_i (i = 1, \ldots, 6)$. We define the perfect IQL $\mathcal{K}$ as the subset of vectors $\mathbf{X} \in L$ whose complementary vectors $\mathbf{X}' \in E'$ lie in the triacontahedron $C(a) = \Pi'\gamma_6(a)$. This is a three-dimensional polyhedron obtained by projecting the six-dimensional cube

$$\gamma_6(a) = \{(z_1, \ldots, z_6) \in \mathbf{R}^6 : -a/2 < z_i < a/2, \quad i = 1, \ldots, 6\},$$

of side length a into E' (see [10] for a description and depiction of a triacontahedron). The points of $\mathcal{K}$ are the vertices of the prolate and oblate rhombohedra which together tile E (Amman tiles, [12]). A schematic model K_0 of a perfect static IQC is obtained by placing an atom belonging to a single atomic species (Mn in our numerical calculations) at each vertex of the Amman tiles of $\mathcal{K}$. This model has proved useful for explaining the observed electron diffraction patterns of IQCs [13,14] and for studying the feasibility of ion channeling therein [8]. It may be viewed as a first step in constructing K, the more realistic disordered IQC that we now define.

K belongs to a large class of disordered IQCs considered by Jarić and Nelson [15], which model IQCs in which phonons and phasons are thermalized, or in which the phasons have been quenched at a high temperature and the phonons thermalized at a lower quenching temperature.