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Cross-Lattice Formulation — Applications in Materials Science

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Reciprocal lattice is, widely, used in materials science as well as condensed-matter physics. The expressions of reciprocal-lattice vectors, having dimensions of inverse of length vary with use of different systems of units. In order to counter this problem, a modified lattice, termed as *cross lattice*, was introduced on **Wednesday, November 8, 1978** during the All Pakistan Mathematical Conference, NED University of Engineering and Technology, Karachi, Pakistan, November 6-8, 1978 (it would be of interest that the formulation was first proposed in an assignment submitted a year earlier by the speaker to Professor Dr. S. A. Husain as part of the course requirement, entitled 'Solid-State Physics') and published as a peer-reviewed paper entitled "A Dimensionless Reciprocal Lattice". The cross-lattice vectors were constructed in such a way that they became independent of the coördinate mesh (system) chosen[ν]. A coördinate-independent representation is a prerequisite of representing generalized laws and forms the basis of principle of general covariance — this was the motivation to present the most general coördinate transformations (the scaled-Poincaré transformations) on **Tuesday, May 12, 2009**. Let $\hat{\boldsymbol{a}}_1$, $\hat{\boldsymbol{a}}_2$, $\hat{\boldsymbol{a}}_3$, be the basis vectors for ordinarty lattice. Any vector $\boldsymbol{L}$, may be represented in terms of these linearly-independent bases $\boldsymbol{L} = L_k \hat{\boldsymbol{a}}_k$ (repeated indices denote summation according to the Einstein convention; all latin indices take up the values 1, 2, 3). The recipriocal-latttice vectors for a nonrectangular lattice, may be constructed, using the basis vectors

$$\hat{\boldsymbol{g}}_k = \in_{klm} \frac{\hat{\boldsymbol{a}}_l \times \hat{\boldsymbol{a}}_m}{2\hat{\boldsymbol{a}}_1 \bullet \hat{\boldsymbol{a}}_2 \times \hat{\boldsymbol{a}}_3}$$

as $\boldsymbol{G} = G_k \hat{\boldsymbol{g}}_k = 2\pi n_k \hat{\boldsymbol{g}}_k$ ($\in_{klm}$ is the Levi-Civita symbol — tensor density as per transformation rules; +1 for even permutation of indices, –1 for odd permutation, zero otherwise); the numbers n_k are integers, this condition is obtained by applying the periodicity condition $f(r+L) = f(r)$. The reciprocal lattice vectors satisfy the condition $\hat{\boldsymbol{a}}_i \bullet \hat{\boldsymbol{g}}_j = \delta_{ij}$; where δ_{ij} is Knoecker delta (1 if the indices match in value, zero otherwise). A cross product of the direct- and the rciprocal-lattice vectors is dimensionless, and named as *cross lattice*, $\hat{\boldsymbol{e}}_i = \hat{\boldsymbol{a}}_i \times \hat{\boldsymbol{g}}_i$ (no summation over i). The cross-lattice length can be written as $\boldsymbol{D} = D_k \hat{\boldsymbol{e}}_k = 2\pi n_k \hat{\boldsymbol{e}}_k$. The following results can, easily, be derived from the above definition, $\boldsymbol{D} \bullet \boldsymbol{L} = \boldsymbol{D} \bullet \boldsymbol{G} = 0$; $exp(i\boldsymbol{D} \bullet \boldsymbol{L}) = exp(i\boldsymbol{D} \bullet \boldsymbol{G}) = 1$ ($i = \sqrt{-1}$). The eigenfunctions of cross lattice can be obtained by considring an anisotropic potential, which depends on angle, θ. The band must be well separated to make non-diagonal matrix elements vanish with respect to band index. Defining a modified Brillouin zone to be a Wigner-Seitz cell in cross lattice and letting $\boldsymbol{D}$ take all values inside this zone, all the coefficients vary and become functions of $\boldsymbol{D}$. However, because of the periodicity in the momentum space, they are all identical functions of $\boldsymbol{D}$, translated in cross-lattice space. Wannier functions, introduced by Gregory H. (Hugh) Wannier (1911-1983) in 1937, are useful for systems, which are *isotroptic*, but *inhomogeneous*.The cross eigenfunctions, belonging to eigenstates of angular momentum in the cross-lattice representation (in quantum mechanics, momentum eigenfunctions represent the wave function of a particle, when it is in a state of definite momentum), are useful for systems, which are *homogeneous*, but *anisotropic*. Such systems are found in liquid crystals. We, now, have the necessary techniques availble to study these systems. Future work may involve mathematical derivation of eigenfunctions, which are both *inhomogeneous* and *anisotropic*. Application of mathematical techniques to problems in materials science, in particular, study of liquid crystals, analysis of diffraction patterns, modeling of electronic-band structures, prediction of interface stability, may bring out new avenues of research, forming the basis of *condensed-matter mathematics*, the term introduced on **Friday, December 28, 2012** during the International Conference on Condensed-Matter Physics and Engineering, Department of Physics, Bahauddin Zakariya University, Multan, Pakistan, December 27-29, 2012. In the field of biomechanics the cross-lattice-structure-based model of human spinal column was put forward in 2019.

*Keywords***:** Condensed-matter mathematics • Liquid crystals • Momentum eigenfunctions • Reciprocal lattice • Wannier functions

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[χ] throughout **First-Class-First-Position** holder; recipient of **4 Gold Medals**; **prize** in *Object Drawing* in Intermediate Grade Drawing Examination, Inspector of Drawing and Art Sindh, Directorate of Education, Hyderabad Region, Sindh; listed in Marquis' Who's Who in the World (15th ed.), Marquis' Who's Who in Asia (1st ed.), Marquis' Who's Who in Science and Engineering (10th ed.), Dictionary of International Biography (27th ed.) and 2000 Outstanding Intellectuals of the Twenty-First Century (1st ed.); Google Scholar • *homepage* • *vita*

[μ] **100% marks in all subjects** during the final semester; **topped the list of the entire student body** receiving master's degrees from University of Karachi during that academic year

[ν] the word *mesh* is used in the spirit that the unit vectors, $(\hat{\boldsymbol{e}}_1, \hat{\boldsymbol{e}}_2, \hat{\boldsymbol{e}}_3)$, along the *x* axis, the *y* axis and the *z* axis, respectively, are related through the orthonormality conditions

$$\hat{\boldsymbol{e}}_i \times \hat{\boldsymbol{e}}_j = \in_{ijk} \hat{\boldsymbol{e}}_k$$

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