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Cross Lattice: A Dimensionless-Reciprocal Lattice for Condensed-Matter Physics

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Reciprocal lattice is, widely, used in condensed-matter physics and materials science. The expressions of reciprocal-lattice vectors, having dimensions of inverse of length, are changed, when different systems of units are used. In order to alleviate this problem, a modified lattice, termed as *cross lattice*, was introduced <https://www.ngds-ku.org/Presentations/Cross.pdf> in 1978 and a complete mathematical formulation published <https://www.ngds-ku.org/Papers/J07.pdf> in 1988. The cross-lattice vectors are constructed in such a way that they became independent of the coordinate system chosen. Let $\hat{a}_1, \hat{a}_2, \hat{a}_3$, be the basis vectors for ordinary lattice. Any vector L , may be represented in terms of these linearly-independent bases $L = L_k \hat{a}_k$ (repeated indices denote summation according to Einstein convention; all latin indices take up the values 1, 2, 3). The reciprocal-lattice vectors for a non-rectangular lattice, may be constructed, using the basis

$$\hat{g}^k = \epsilon_{klm} \frac{\hat{a}_l \times \hat{a}_m}{2\hat{a}_l \cdot \hat{a}_2 \times \hat{a}_3}$$

as $G = G_k \hat{g}^k = 2\pi n_k \hat{g}^k$; the numbers n_k are integers, ϵ_{klm} is Levi-Civita symbol, whose values are +1, when the indices form even permutation (123, 231, 312), -1, when the indices form odd permutation (132, 213, 321) and zero otherwise (one or more indices repeated). The equation defining \hat{g}^k is obtained by applying the periodicity condition $f(r+L) = f(r)$. The reciprocal lattice vectors satisfy the orthonormality condition $\hat{a}_i \cdot \hat{g}_j = \delta_{ij}$; where δ_{ij} is Kronecker delta, whose value is 1 when $i = j$ and zero otherwise. A cross product of the direct- and the reciprocal-lattice vectors is dimensionless, and named as *cross lattice*, $\hat{e}_i = \hat{a}_j \times \hat{g}_k$ (no summation over i). The cross-lattice length can be written as $D = D_k \hat{e}_k = 2\pi n_k \hat{e}_k$.

These results can, easily, be derived from the given definition $D \cdot L = D \cdot G = 0$; $\exp(iD \cdot L) = \exp(iD \cdot G) = 1$, ($i = \sqrt{-1}$). The eigenfunctions of cross lattice can be obtained by considering 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 D take all values inside this zone, all the coefficients vary and become functions of D . However, because of the periodicity in the momentum space, they are all identical functions of D , translated in cross-lattice space. Wannier functions are useful for systems, which are *isotropic*, but *inhomogeneous*. The cross eigenfunctions, belonging to eigenstates of angular momentum in cross-lattice representation, are useful for systems, which are *homogeneous*, but *anisotropic*. At present, our research group is engaged in the following projects — (a) application of cross-lattice formulation to liquid-crystal structure, (b) crystal-structure concepts applied to static and dynamic modeling of the human-spinal column, (c) cross-lattice-structure-based modeling of the human spinal column and (d) mathematical derivation of eigenfunctions, which are both *inhomogeneous* and *anisotropic*. Some preliminary results of (a) and (b) may be available next year and (c) by the end of this decade. This paper is dedicated to the loving memory of my dearest teacher and mentor, **Professor Dr. S. A. (Shaikh Ansar) Husain** (born: 1933; passed away: 2011). Prof. Husain obtained his BSc from Lucknow University, India (1952), MSc from University of Karachi (1955) and PhD from University of Alberta, Canada (1968) after obtaining another MSc from that university in 1965. He served Department of Physics, University of Karachi during 1955-1993 (Lecturer 1955-1958; Assistant Professor 1958-1969; Associate Professor 1969-1979; Professor 1979-1993; Chairman during 1970s, 1980s and 1990s; Secretary, Affiliation Committee 1979-1987). He was author of physics textbooks for HSC and BSc. The speaker had the honor to share authorship with his beloved teacher in 7 peer-reviewed journal papers (a dimensionless-reciprocal lattice^a, spacetime representation of global-electrocortical activity^b, behavior of massive particles near the velocity of light^c, effects of weak magnetic fields on global-electrocortical activity^d, effects of weak electromagnetic fields on global-electrocortical activity^e, group structure of a covariant model of global-electrocortical activity^f and EEG in weightlessness: a theoretical estimate^g) and 7 conference presentations (relativistically-streaming plasmas containing dyons^h, cross lattice and eigenfunctionsⁱ, 2×2 representations of REMO for bradyons^k, 4×4 representation of REMO for bradyons^l, luxon-bradyon transformation^m, a generalization of the covariant-effective-mass tensorⁿ and effective mass in the relativistic range^o). Department of Physics, University of Karachi, organized a function in 2006 to celebrate the achievements of the legendary professor (Fig. 1).

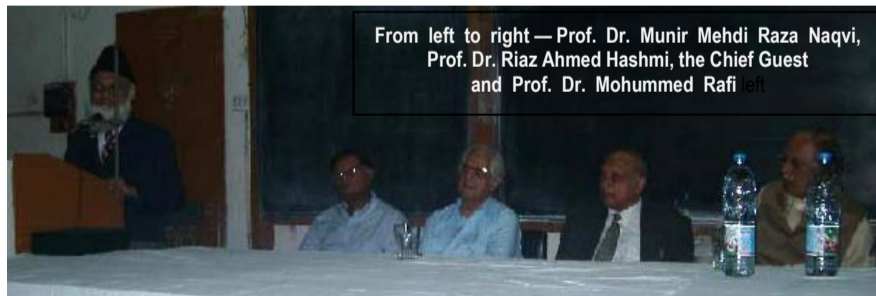


Fig. 1 On August 31, 2006, the speaker was paying tribute to his mentor on the occasion of celebrating the achievements of Prof. Dr. S. A. Husain (seated second from right) in Department of Physics, University of Karachi

Keywords: Brillouin zone • Momentum eigenfunctions • Wannier functions • Wigner-Seitz cell

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^a<https://www.ngds-ku.org/Papers/J07.pdf>

^b<https://www.ngds-ku.org/Papers/J08.pdf>

^c<https://www.ngds-ku.org/Papers/J10.pdf>

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