von NEUMANN LATTICES and WANNIER FUNCTIONS

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Abstract:

In his celebrated book "Mathematical Foundations of Quantum Mechanics," von Neumann introduced the notion of a lattice in the phase plane [1]. This lattice has a unit cell of area h, the Planck constant, and is of wide use both in physics and in signal processing, where it is called the Gabor lattice[2]. One can construct such a

phase space lattice by using the elementary shift operators $T(a) = \exp\left(\frac{i}{\hbar}pa\right)$ and $\tau\left(\frac{2\pi}{a}\right) = \exp\left((ix\frac{2\pi}{a})\right)$. These operators commute and they determine the *kq*-

representation[3]. The k and q are the symmetric coordinates for periodic potentials. In solids of much importance are the Wannier functions, which is an orthonormal set of functions on a crystalline lattice in configuration space[4]. They play an important role in the magnetic field problem, where one can assign a von Neumann lattice to each Landau level. In his book [1] von Neumann constructed a set of coherent states

on a lattice in phase plane by using the shift operators T(a) and $\tau\left(ix\frac{2\pi}{a}\right)$, and stated

without proof that the set he had built was complete and that it could be made orthogonal. The completeness part of his statement was first proven about 40 years after the German edition of the von Neumann book[5-7]. The orthogonality part of von Neumann's statement has taken a fascinating turn in the last 25 years, after 1981, when the Balian-Low theorem appeared. According to this theorem it is impossible to build an orthonormal set of functions by shifting a single function on a von Neumann lattice. An idea to bypass the Balian-Low theorem was raised by Wilson and coworker in a numerical iteration procedure[8]. This procedure was later complemented by an analytic construction by Daubuchies et al.[9].

More recently[10], a symmetry framework was developed for a unique assignment of an orthonormal basis on a von Neumann lattice. This basis can be interpreted as having the meaning of Wannier functions on a phase plane.

References

[1] J. von Neumann, Mathematical Foundations of Quantum Mechanics (Princeton University Press, 1955) pp 406, 407

[2] D. Gabor, J. Inst. Electron. Eng. 93,429(1946).

[3] J. Zak, Phys. Rev.Lett.19, 1385(1967); J. Zak, Phys. Today, 23, 51 (1970).

[4] G. Wannier, Phys. Rev. 52, 191(1937).

[5] A.M. Perelomov, Theor.Math. Phys. 6, 156(1971)

[6] V. Bargmann, P. Butera, L. Girardello and J.R. Klauder, Rep. Math. Phys. 2, 221(1971).

7. H. Bacry, A. Grossmann, and J. Zak, Phys. Rev B12, 1118 (1975).

8. K.G. Wilson, Generalized Wannier Functions, Cornell University Preprint; D.J.

Sullivan, J.J. Rehr, J.W. Wilkins, and K.G. Wilson, Phase Space Wannier Functions in Electronic Structure Calculations, Cornell University Preprint.

[9] I. Daubechies, S. Jaffard, and J.L. Journes, SIAM J. Math. Anal. 22, 559 (1991).

[10] J. Zak, J.Phys. A: 35, L369, (2002); ibid 36, L553 (2003).