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von Neuman Lattices and Wannier Functions

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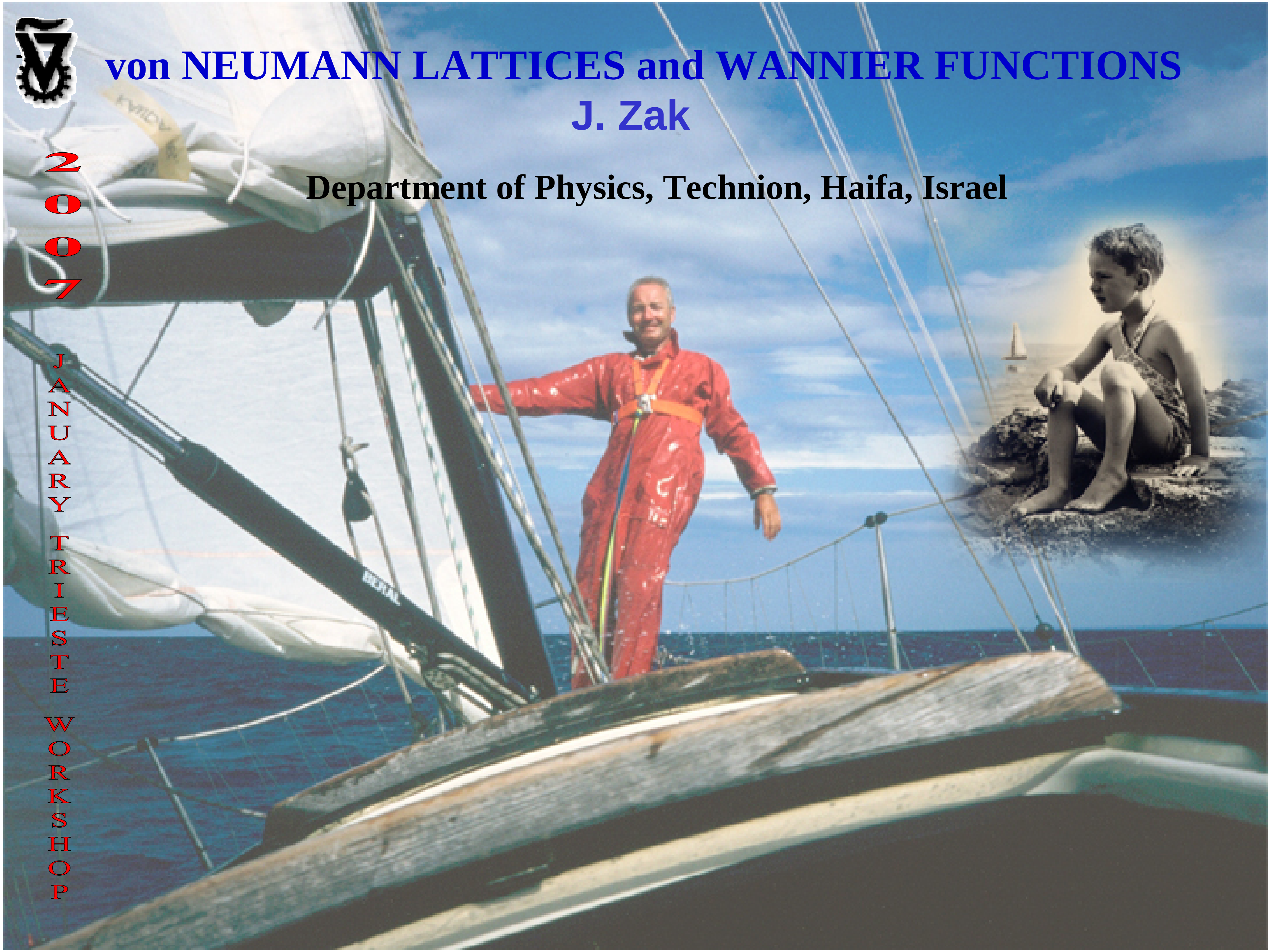


von NEUMANN LATTICES and WANNIER FUNCTIONS

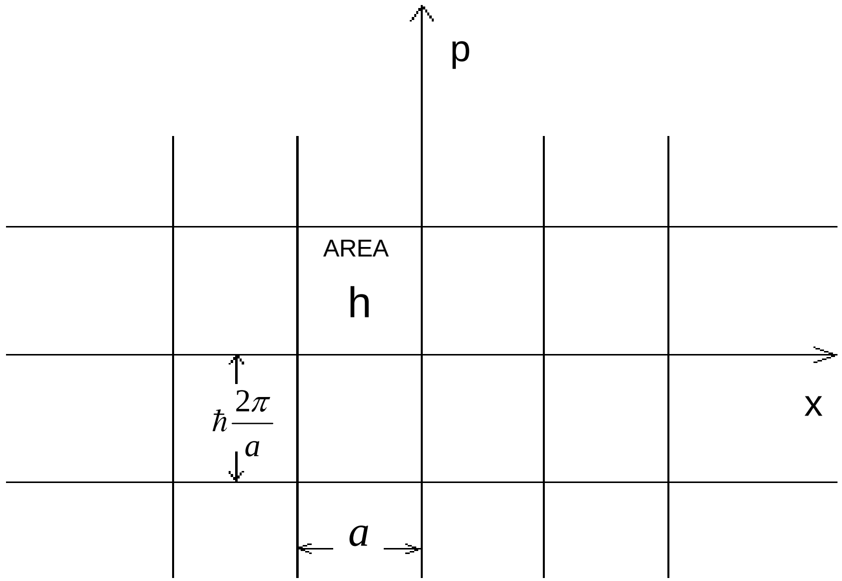
J. Zak

Department of Physics, Technion, Haifa, Israel

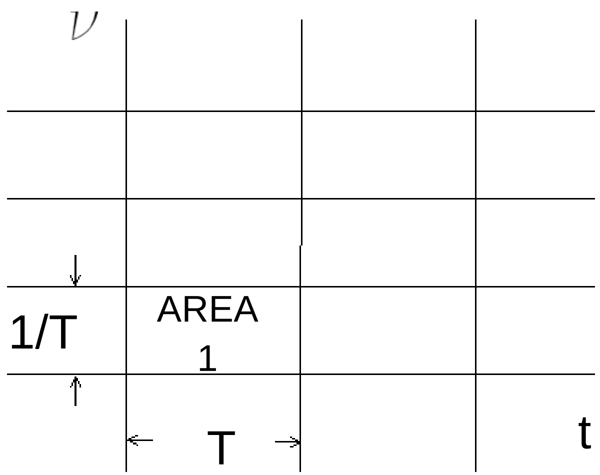
OUTLINE:

1. **SYMMETRIC COORDINATES IN SOLIDS**
2. **von NEUMANN LATTICES (1931) [Dennis Gabor (1946)] and SETS.**
3. **EXAMPLE :COHERENT STATES.**
4. **BALIAN-LOW THEOREM**
5. **WANNIER FUNCTIONS IN THE PHASE PLANE**

- **TRIESTE WORKSHOP, JANUARY 11-13, 2007**



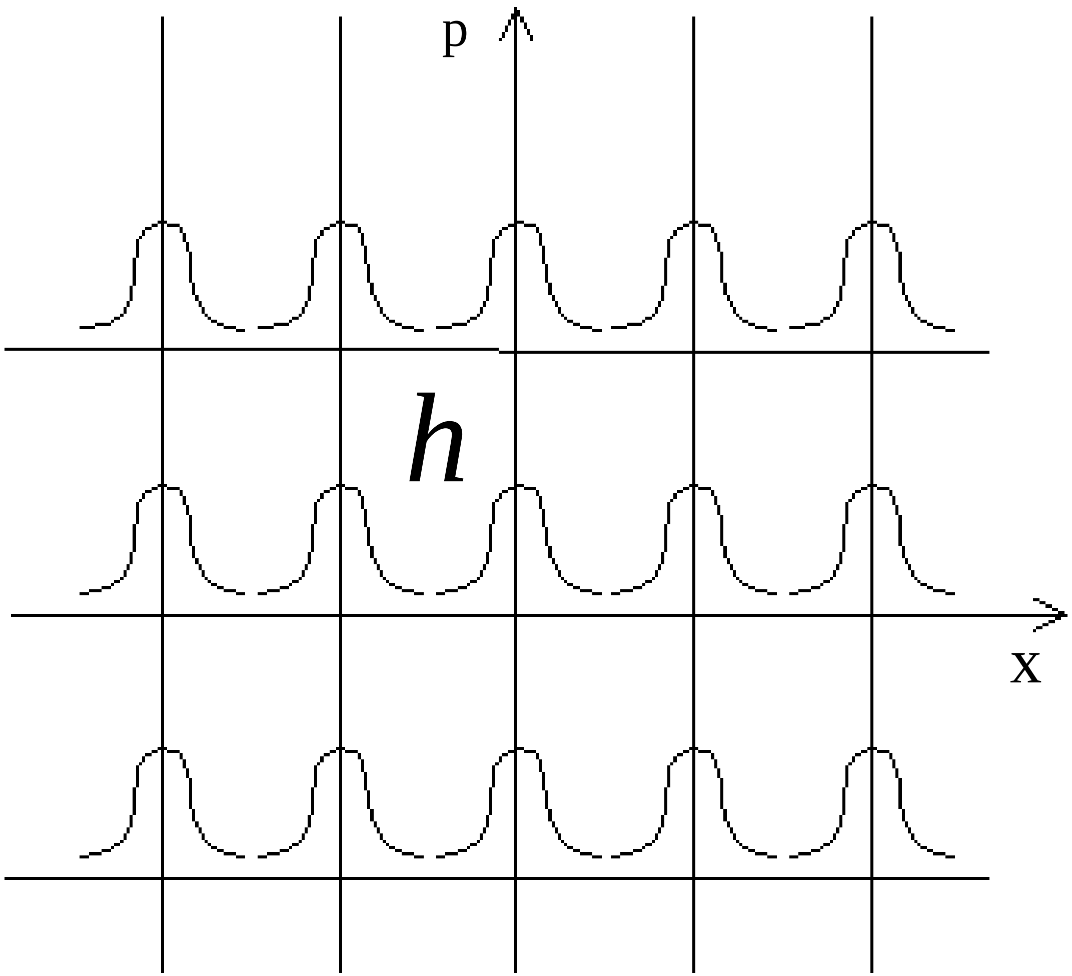
von NEUMANN'S LATTICE (1931)



D.GABOR, J.Inst.Elrctron.Eng. 93, 429 (1946)

von NEUMANN'S SET

$$\bar{\mathrm{p}} = \hbar \frac{2\pi}{a} n$$



$$\bar{x} = ma$$

1. SYMMETRIC COORDINATES IN SOLIDS

In atomic physics:

In solids: $$V(\vec{r}) = V(|\vec{r}|) : r, \vartheta, \varphi$$

$$V(x) = \sum_n V_n \exp\left(i \frac{2\pi}{a} xn \right) \quad : \quad \exp\left(i \frac{2\pi}{a} x \right)$$

$$\exp\left(\frac{i}{\hbar} pa \right) : \exp(ika) \qquad 0 \le k \le \frac{2\pi}{a} \qquad \text{(A)}$$

$$\exp\left(ix \frac{2\pi}{a} \right) : \exp\left(iq \frac{2\pi}{a} \right) \qquad 0 \le q \le a$$

k and *q* symmetric coordinates in solids

k- conserved crystal momentum

q – the periodic potential energy depends on *q* only.

The operators in (A) form a complete set of commuting operators.

They define the *kq*- representation:

$$x = i\frac{\partial}{\partial k} + q, \qquad p = -i\hbar\frac{\partial}{\partial q}$$

$$C(k,q) = \left(\frac{a}{2\pi}\right)^{1/2} \sum_n \exp(ikan)\psi(q - na)$$

$$\psi(x) = \left(\frac{a}{2\pi}\right)^{1/2} \int_{BZ} C(k,x)dk$$

THREE BASIC REPRESENTATIONS IN QUANTUM MECHANICS

- 1. *x*-representation*:* $x\ ,\ p = -i\hbar \frac{\partial}{\partial x}\ , \psi(x)$

- *2.* *p*-representation: $x = i\hbar \frac{\partial}{\partial p}\ ,\ p\ ,\ F(p)$

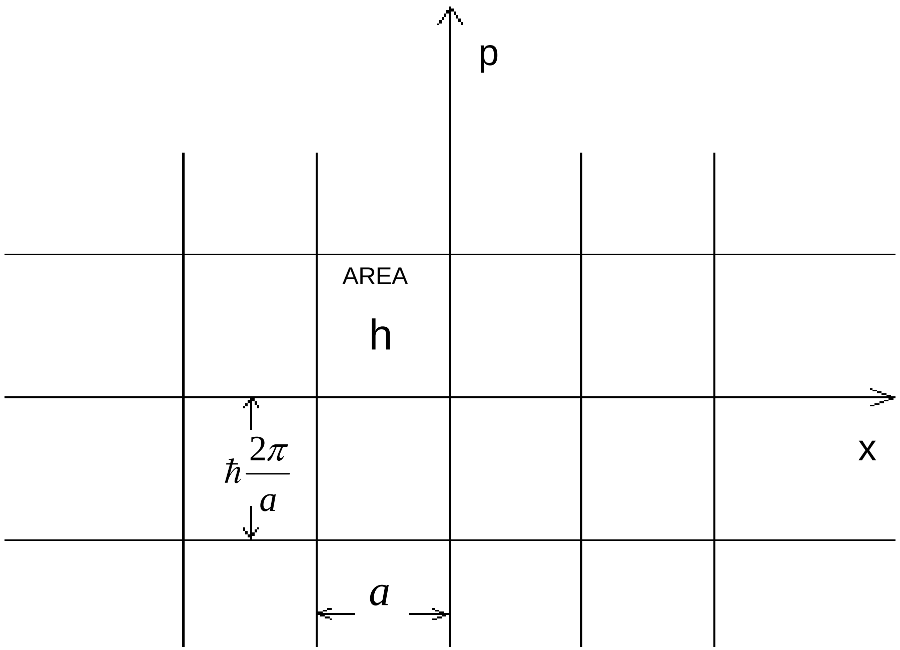
$$F(p) = \frac{1}{(2\pi\hbar)^{1/2}} \int \exp\left(-\frac{i}{\hbar} px \right) \psi(x) dx$$

- *3. kq-representation* $x = i\frac{\partial}{\partial k} + q\ ,\ p = -i\hbar\frac{\partial}{\partial q}\ ,\ C(k,q)$

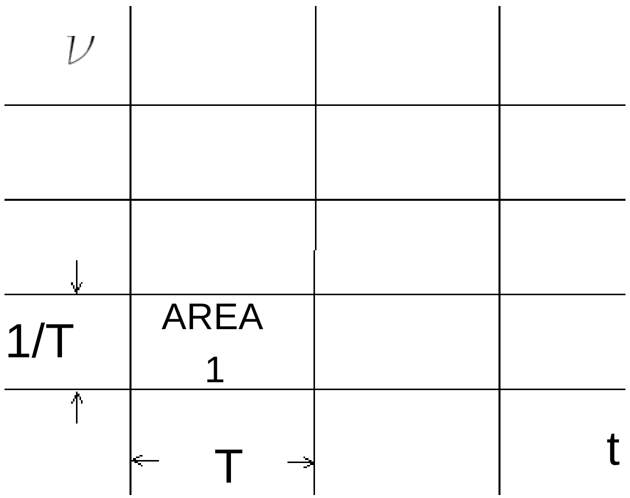
$$C(k,q) = \left(\frac{a}{2\pi}\right)^{1/2} \sum_n \exp(ikan)\psi(q - na)$$

$$C\left(k + \frac{2\pi}{a}, q\right) = C(k,q) = \exp(-ika)C(k, q + a)$$

$$\psi(x) = \left(\frac{a}{2\pi}\right)^{1/2} \int C(k,x)dk$$



von NEUMANN'S LATTICE (1931)



D.GABOR, J.Inst.Elrctron.Eng. 93, 429 (1946)

3. EXAMPLE: COHERENT STATES AND von NEUMANN'S SETS

$$\psi_0(x) = \left(\frac{1}{\pi\lambda^2}\right)^{1/4} \exp\left(-\frac{x^2}{2\lambda^2}\right)$$

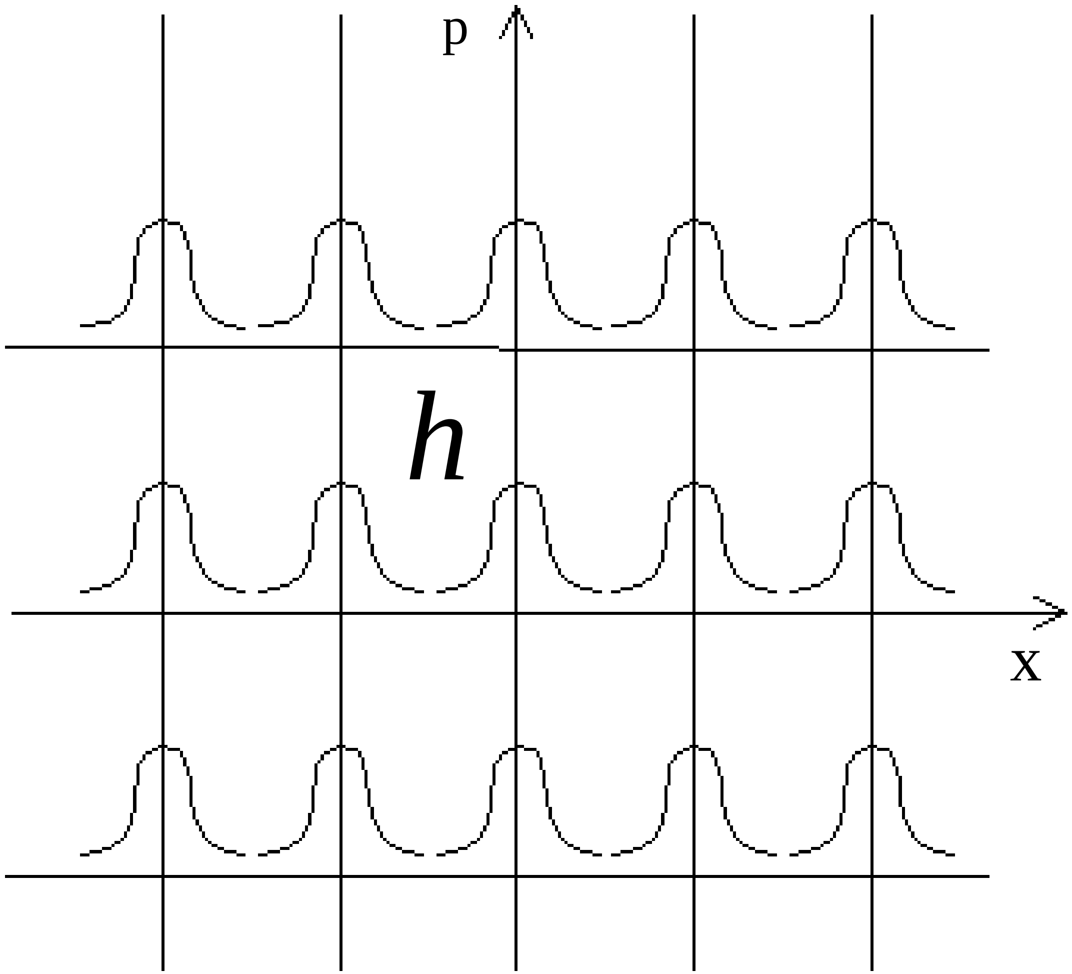
Coherent state

$$\psi_{\bar{x}\,\bar{p}}(x) = D(\bar{x},\bar{p})\psi_0(x) = \exp(-\frac{i}{2\hbar}\bar{x}\,\bar{p})\exp\left(\frac{i}{\hbar}\bar{p}x\right)\psi_0(x-\bar{x})$$

$$D(\bar{x},\bar{p}) = \exp\left(-\frac{i}{2\hbar}\bar{x}\,\bar{p}\right)\exp\left(\frac{i}{\hbar}\bar{p}x\right)\exp\left(-\frac{i}{\hbar}\bar{x}p\right)$$

von NEUMANN'S SET

$$\bar{p} = \hbar \frac{2\pi}{a} n$$



$$\bar{x} = ma$$

3. Von NEUMANN'S SET IN THE kq-REPRESENTATION

$$\psi_{mn}(x) = (-1)^{mn} \exp\left(i \frac{2\pi}{a} n\, x \right) \psi_0(x - ma)$$

$$C_{mn}(k,q) = (-1)^{mn} \exp\left(i \frac{2\pi}{a} nq - ikma \right) C_0(k,q)$$

$$C_0(k,q) = \left(\frac{2\pi}{a} \right)^{1/2} \sum_{l=-\infty}^{\infty} \exp(ikal)\psi_0(q - la) =$$

$$= \left(\frac{a^2}{4\pi^3\lambda^2} \right)^{1/4} \exp\left(-\frac{q^2}{2\lambda^2} \right) \theta_3\left(\frac{ka}{2} - i\frac{qa}{2\lambda^2} \middle| i\frac{a^2}{2\pi\lambda^2} \right)$$

Jacobi Theta Function

$$\theta_3(z \,|\, \tau) = \sum_{l=-\infty}^{\infty} \exp(2izl + i\pi\tau l^2)$$

4. BALIAN-LOW THEOREM

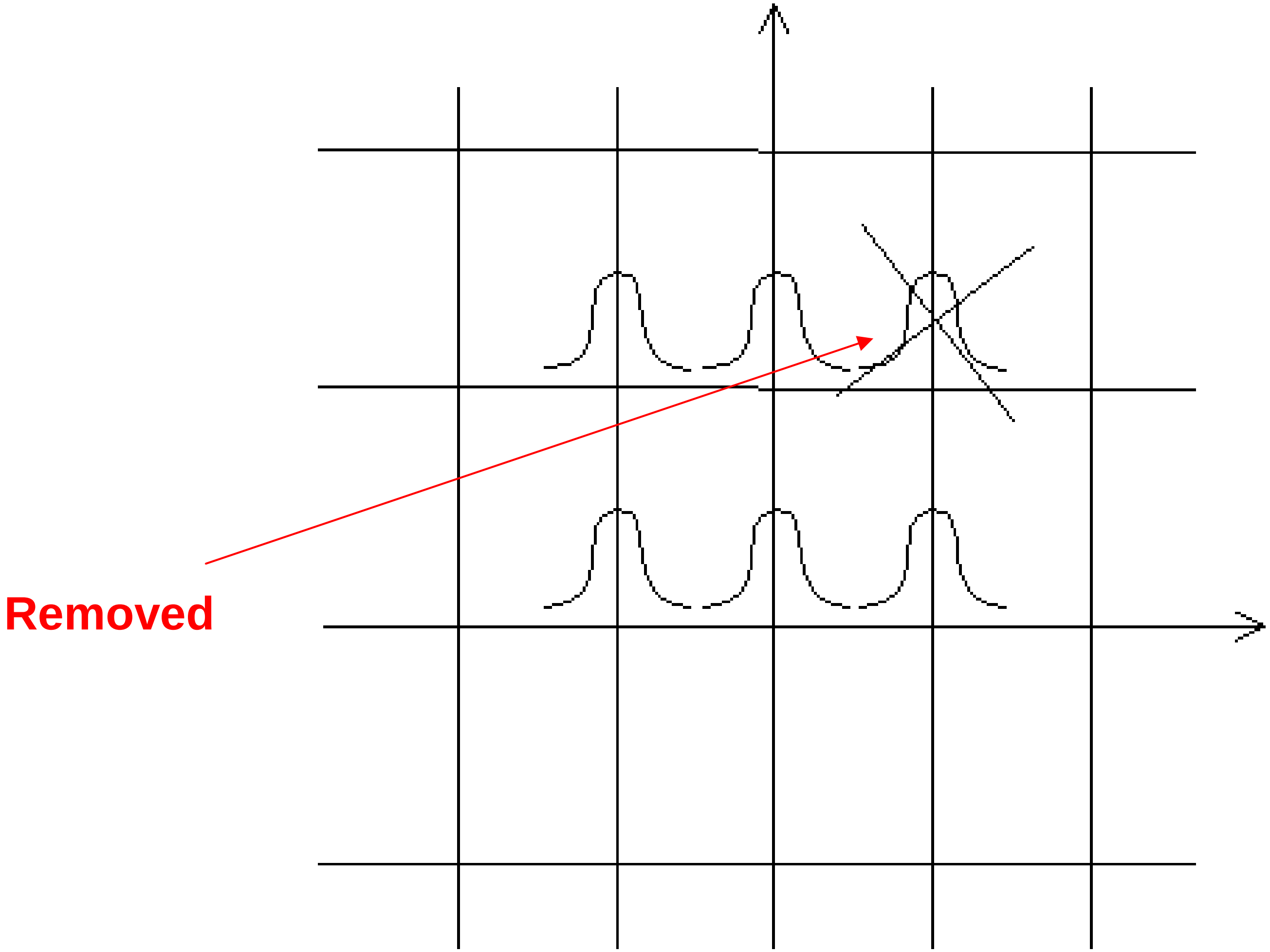
4a. Completeness of von Neumann's Set

If from
$$\int C(k,q)C_0^*(k,q)\exp\left(ikam - iq\frac{2\pi}{a}n\right)dkdq = 0$$

It follows
$$C(k,q) = 0$$

then the set
$$C_0(k,q)\exp\left(-ikam + iq\frac{2\pi}{a}n\right)$$

is complete.



A.M. Perelomov, Teor. Mat. Fiz. 6,213(1971)

4c. Orthogonality of von Neumann's Set

$$\left|\langle \alpha_{mn} | \alpha_{m'n'} \rangle\right|^2 =$$

$$= \left| \iint \left| C_0(k,q) \right|^2 \exp[-ika(m'-m) + iq\frac{2\pi}{a}(n'-n)]dkdq \right|^2$$

$$\left| \alpha_{mn} \rangle = D\left(ma, n\frac{2\pi}{a}\hbar \right) \right| 0 \rangle$$

4d. Generalized von Neumann's Set

$$\psi_{mn}(x) = D\left(ma, n\hbar\frac{2\pi}{a}\right)\psi(x)$$

$$C_{mn}(k,q) = (-1)^{mn}\exp(-ikam + iq\frac{2\pi}{a}n)C(k,q)$$

$$\langle C_{mn}(k,q), C_{m'n'}(k,q)\rangle =$$

$$\iint \left|C(k,q)\right|^2 \exp\left[-ika(m'-m) + iq\frac{2\pi}{a}(n'-n)\right]dkdq$$

For $\left|C(k,q)\right|^2 = const$

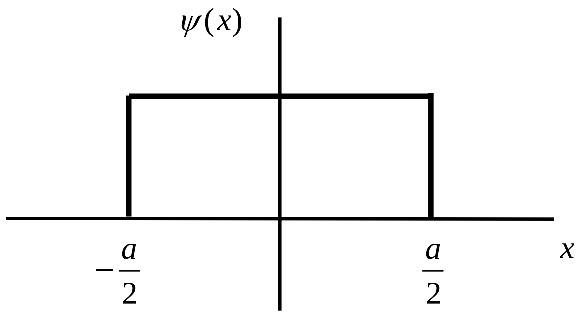
$C_{mn}(k,q)$ is an orthonormal set.

V. Bargmann, P. Butera, L. Girardello, and J.R. Klauder, Rep. Math. Physics2, 221(1971)

H. Bacry, A. Grossmann and J.Z. Phys. Rev. B 12, 1118(1975)

EXAMPLE

$$\psi(x)=\begin{cases}\dfrac{1}{\sqrt{a}} & |x|<\dfrac{a}{2}\\[2ex] 0 & |x|>\dfrac{a}{2}\end{cases}$$



$$C(k,q)=\frac{1}{\sqrt{2\pi}}$$

R. Balian, C.R. Acad.Sc.,Paris 292, 1357(1981)

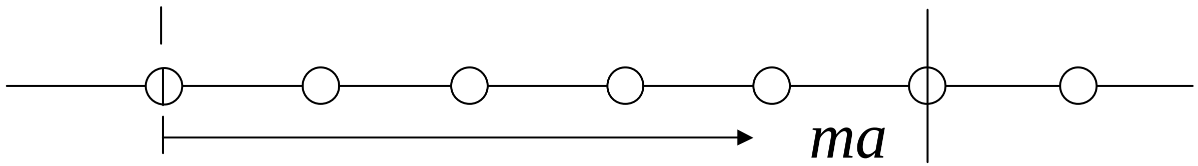
$$\Delta x=\frac{a}{\sqrt{12}} \quad , \quad \Delta p=\infty$$

F. Low, In Passion for Physics- Essays in Honor of Geoffrey Chew, Ed C. DeTar et al (Singapor: World Scientific), page 17 (1985)

Balian-Low Theorem:

5. WANNIER FUNCTIONS

5.1 One-dimensional crystal



$$w_{lm}(x) \equiv w_l(x-ma) = \left(\frac{a}{2\pi}\right)^{\frac{1}{2}} \int_{BZ} \psi_{lk}(x)\exp(-ikam)dk$$

Wannier function in the kq-representation

$$\boxed{\begin{aligned} w_{lm}(k,q) &= \left(\frac{a}{2\pi}\right)^{1/2} \sum_s \exp(ikas)\, w_l(q-ma-sa) = \\ &= \exp(-ikam)\,\psi_{lk}(q) \end{aligned}}$$

5.3 MOVITAVATION FOR PHASE PLANE WANNIER FUNCTIONS – THE MAGNETIC FIELD PROBLEM

$$H = \frac{1}{2m}\left(\vec{p} + \frac{e}{2c}\vec{B}\times\vec{r}\right)^2$$

$$\vec{v} \quad = \frac{1}{m}\left(\vec{p} + \frac{e}{2c}\vec{B}\times\vec{r}\right) = \frac{1}{m}\left(\vec{p} - \frac{e}{2c}\vec{B}\times\vec{r}\right) + \frac{e\vec{B}}{mc}\times\vec{r} = \vec{\omega}\times(\vec{r} - \vec{r}_o)$$

$$-\vec{\omega}\times\vec{r}_o = \frac{1}{m}\left(\vec{p} - \frac{e}{2c}\vec{B}\times\vec{r}\right)$$

$$\vec{\omega} = \frac{e\,\vec{B}}{mc}$$

The orbit center $\vec{r}_o$

It is a conserved quantity, because one can check:

$$\vec{\pi} = \vec{p} + \frac{e}{2c}\vec{B}\times\vec{r} \ commutes\ with\ \vec{\pi}_o = \vec{p} - \frac{e}{2c}\vec{B}\times\vec{r}$$

$$\pi_x = p_x - \frac{eB}{2c}y \qquad\qquad \vec{\pi}_{ox} = \vec{p}_x + \frac{e}{2c}y : y_0$$

$$\pi_y = p_y + \frac{eB}{2c}x \qquad\qquad \vec{\pi}_{oy} = \vec{p}_y - \frac{e}{2c}x : x_0$$

22

Orbit Center $\vec{r}_o$ **and the phase plane X, P**

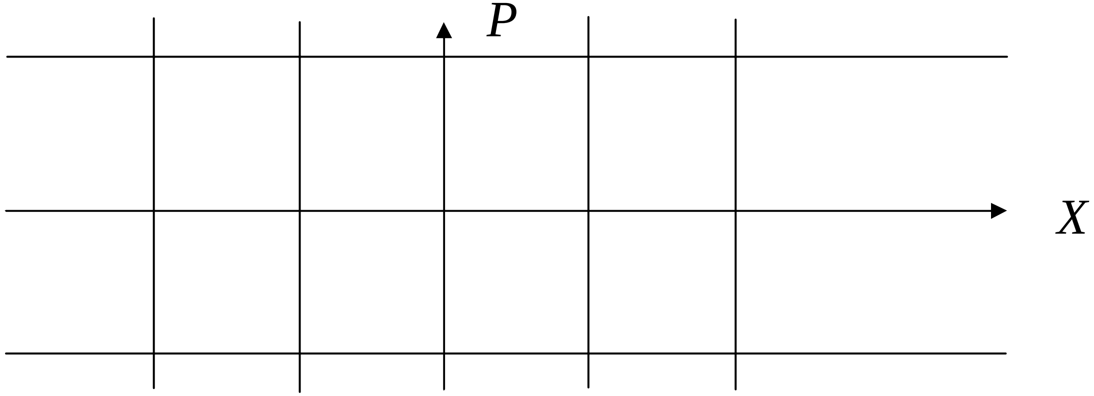
$$-\vec{\omega}\times\vec{r}_o = \frac{1}{m}\left(\vec{p} - \frac{e}{2c}\vec{B}\times\vec{r}\right)$$

$$x_0 = \frac{1}{2}x - \frac{p_y}{m\omega} \equiv X$$

$$\rightarrow \quad [X, P] = i\hbar$$

$$y_0 = \frac{1}{2}y + \frac{p_x}{m\omega} \equiv \frac{P}{m\omega}$$

X and P form a phase plane



von Neuman lattice of the orbit center

Orthogonalization on a lattice In Configuration Space

Given $\psi(x)$, we define a Bloch-like function $\phi_k(x)$

$$\phi_k(x) = \sum_n e^{ikan}\psi(x-na)$$

Then there are 2 ways to define a normalized Bloch-like function $\psi_k(x)$ such that

$$\int_{UC} \left|\psi_k(x)\right|^2 dx = \frac{a}{2\pi}$$

UC $\equiv$ Unit Cell

1. $$\psi_k(x) = \left(\frac{a}{2\pi}\right)^{1/2} \frac{\phi_k(x)}{s^{1/2}(k)},$$ where

$$s(k) = \int_{UC} \left|\phi_k(x)\right|^2 dx$$

2. $$\psi_k(x) = \frac{\phi_k(x)}{S^{1/2}(k,x)},$$ where

$$S(k,x) = \pi\left[\left|\phi_k(x)\right|^2 + \left|\phi_k\left(x - \frac{a}{2}\right)\right|^2\right]$$

In both cases we have:

Wannier functions

$$w(x-ma)=\left(\frac{a}{2\pi}\right)^{1/2}\int_{BZ}\psi_k(x-ma)\,dk$$

$$\int w^*(x-ma)\,w(x-m'a)\,dx=\delta_{mm'}$$

WANNIER FUNCTIONS IN PHASE PLANE

In dealing with the problem of macroscopic measurement in quantum mechanics, von Neumann has suggested building a discrete set of coherent states

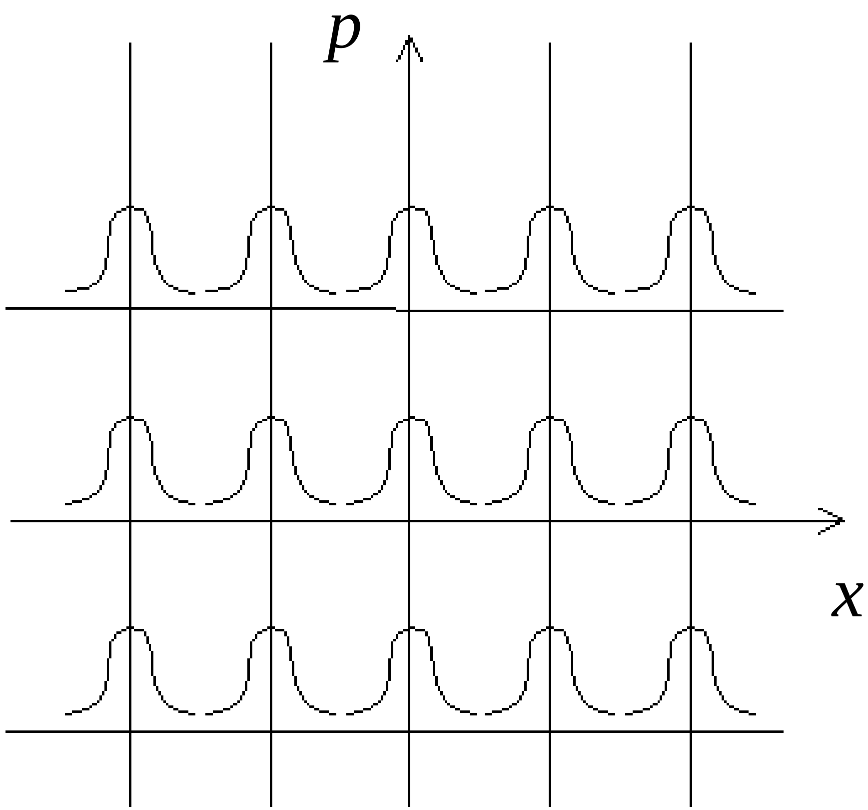
$$\psi_{\ell m}(x) = (-1)^{lm} \exp\left(i \frac{2\pi}{a} x\ell \right) \psi_o(x - ma)$$

The *kq*-transform $C_{\ell m}(k,q)$ of $\psi_{\ell m}(x)$ is

$$C_{\ell m}(k,q) = \exp(-ikam + i\frac{2\pi}{a} q\ell) C_o(k,q)$$

$$C_o(k,q) = \left(\frac{a}{2\pi}\right)^{1/2} \left(\frac{1}{\pi\lambda^2}\right)^{1/4} \exp\left(-\frac{q^2}{2\lambda^2}\right) \theta_3\left(\frac{ka}{2} - i\frac{qa}{2\lambda^2} \,|\, i\frac{a^2}{2\pi\lambda^2}\right)$$

The von Neumann Set



Modified von Neumann’s sets

von Neumann’s set was constructed from a single function on a lattice in phase plane with unit area h, which has led to the Balian-Low theorem. In the signal processing community this is called the “no-go theorem.” There were a number of ideas to by-pass the Balian-Low theorem

K.G. Wilson, Generalized Wannier Functions, 1987, Cornell University preprint

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

JZ, J. Phys. A: Math. Gen. 35, L369 (2002); 36, L553 (2003)

In the latter reference, symmetry arguments were used to construct an orthonormal set on a von Neumann lattice

Define $$\left[\psi_o(x) = \left(\frac{1}{\pi\lambda^2}\right)^{1/4} \exp\left(-\frac{x^2}{2\lambda^2}\right)\right]$$

$$\psi_o^{(even)}(x) = \frac{1}{\sqrt{2}}\left[\psi_o(x) + \psi_o(x - \frac{a}{2})\right] \quad , \quad \left(I \mid \frac{a}{2}\right)\psi_o^{(even)}(x) = \psi_o^{(even)}(x)$$

$$\psi_o^{(odd)}(x) = \frac{1}{\sqrt{2}}\left[\psi_o(x) - \psi_o(x - \frac{a}{2})\right] \quad , \quad \left(I \mid \frac{a}{2}\right)\psi_o^{(odd)}(x) = -\psi_o^{(odd)}(x)$$

$$\psi_{\ell m}(x) = \frac{1}{\sqrt{2}}\left\{ e^{i\frac{2\pi}{a}(x-\frac{a}{4})\ell}\psi_o^{(even)}(x - ma) - e^{-i\frac{2\pi}{a}(x-\frac{a}{4})\ell}\psi_o^{(odd)}(x - ma - \frac{a}{2})\right\}$$

In the *kq*-presentation $\psi_{\ell m}(x)$ becomes

$$C_{\ell m}(k,q)=\frac{1}{\sqrt{2}}e^{-ikam}\left\{e^{i\frac{2\pi}{a}(q-\frac{a}{4})\ell}C_o^{(even)}(k,q)+e^{-i\frac{2\pi}{a}(q-\frac{a}{4})\ell}C_o^{(odd)}(k,q)\right\}=$$

$$=e^{-ikam}\left\{\cos\left[\frac{2\pi}{a}(q-\frac{a}{4})\ell\right]C_o(k,q)+i\sin\left[\frac{2\pi}{a}(q-\frac{a}{4})\ell\right]C_o(k,q-\frac{a}{2})\right\}$$

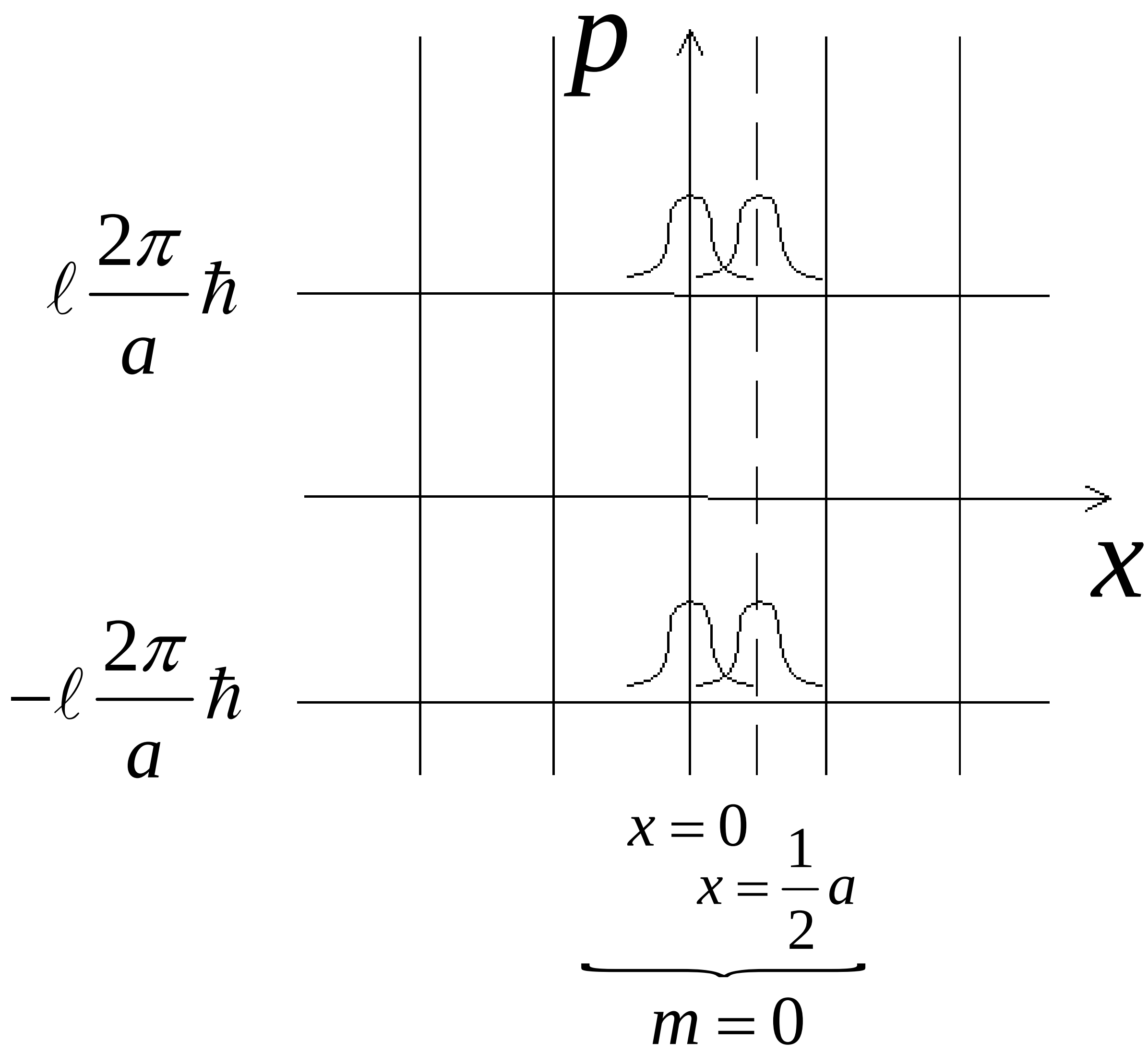
$$\equiv\left\langle k,q\middle|\ell,m\right\rangle$$

These are modified coherent states

Remarks about the orthonormal functions

$$\left|\ell,m\right\rangle=\frac{1}{2}\left\{\begin{array}{l}(-i)^{\ell}\left|ma,\ell\frac{2\pi}{a}\hbar\right\rangle+i^{\ell}\left|ma,-\ell\frac{2\pi}{a}\hbar\right\rangle \\ +\left|(m+\frac{1}{2})a,\ell\frac{2\pi}{a}\hbar\right\rangle-\left|(m+\frac{1}{2})a,-\ell\frac{2\pi}{a}\hbar\right\rangle\end{array}\right\}$$

These are modified coherent states



Schematic plot of the function $\langle x \mid l, 0 \rangle$

$\langle x \mid l, m \rangle$ is a complete set, but not orthogonal

Remarks about the orthonormal functions (continued)

$$w_{\ell m}(k,q) = \frac{\langle k,q|\ell,m\rangle}{S^{1/2}(k,q)}$$

$$S(k,q) = \pi\left[|C_o(k,q)|^2 + |C_o(k,q-\frac{a}{2})|^2\right] =$$

$$= \theta_3\left(\frac{ka}{2}|i\frac{a^2}{4\pi\lambda^2}\right)\theta_3\left(\frac{2\pi q}{a}|i\frac{4\pi\lambda^2}{a^2}\right)$$

$$w_{\ell m}(k,q) = e^{-ikam}\psi_{\ell k}(q)$$

$$\iint w^*_{\ell m}(k,q)w_{\ell' m'}(k,q)dkdq = \delta_{\ell\ell'}\delta_{mm'}$$

The division by $S^{1/2}(k,q)$

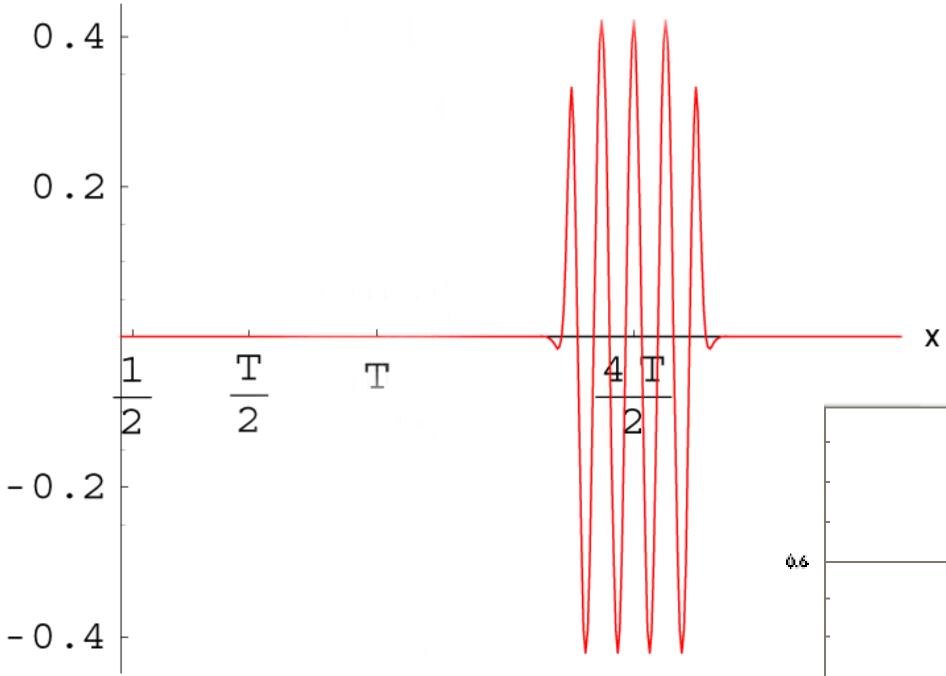
makes the modified coherent states

$\langle k,q|\ell,m\rangle$ orthogonal.

While $|\ell,m\rangle$ is a sum of 4 coherent states, the Wannier functions $w_{\ell m}(k,q)$ is an infinite linear combination of coherent states:

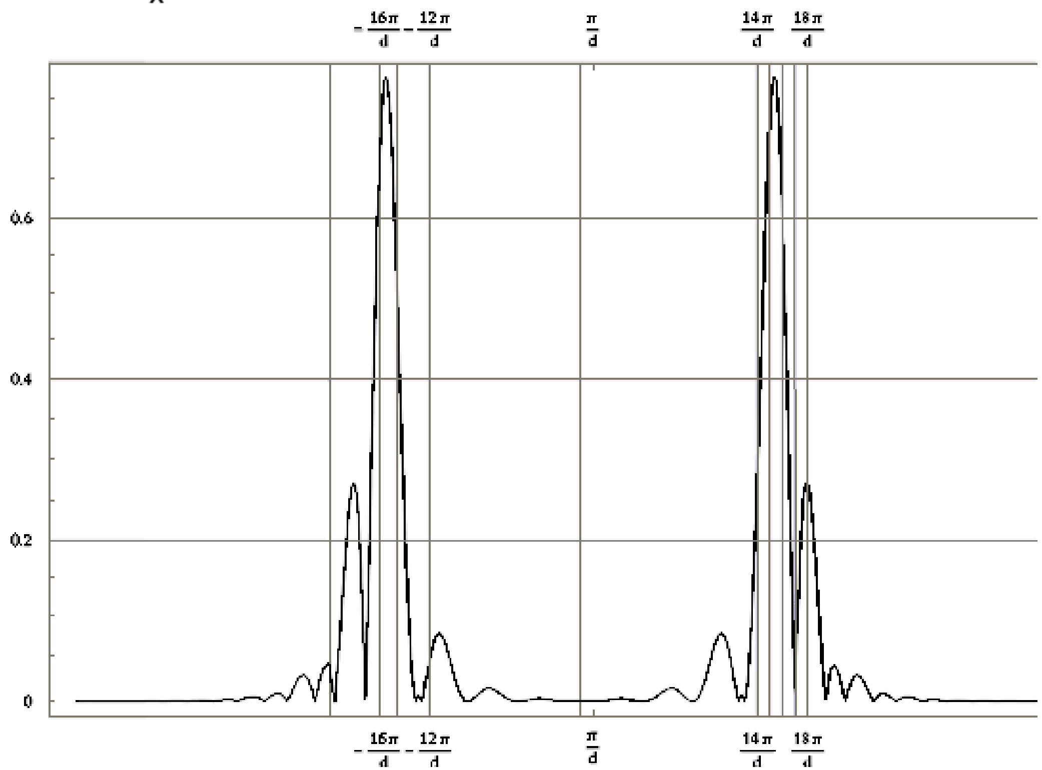
$$\left| w_{\ell m} \right\rangle = \frac{1}{2}\left\{ \begin{array}{l} \sum\limits_{s,t} (-1)^{s\ell} a_{st} \{ (-1)^{\ell} \left| (m+s)a, (\ell+2t)\frac{2\pi}{a}\hbar \right\rangle \\ + i^{\ell} \left| (m+s)a, (-\ell+2t)\frac{2\pi}{a}\hbar \right\rangle + (-1)^{t} \left| \left(m+s+\frac{1}{2} \right) a, (\ell+2t)\frac{2\pi}{a}\hbar \right\rangle \\ - (-1)^{t} \left| \left(m+s+\frac{1}{2} \right) a, (-\ell+2t)\frac{2\pi}{a}\hbar \right\rangle \end{array} \right\}$$

Here: $$\frac{1}{S^{1/2}(k,q)} = \sum_{s,t} a_{st} \exp\left(-ikas + iq\frac{2\pi}{a} 2t \right)$$



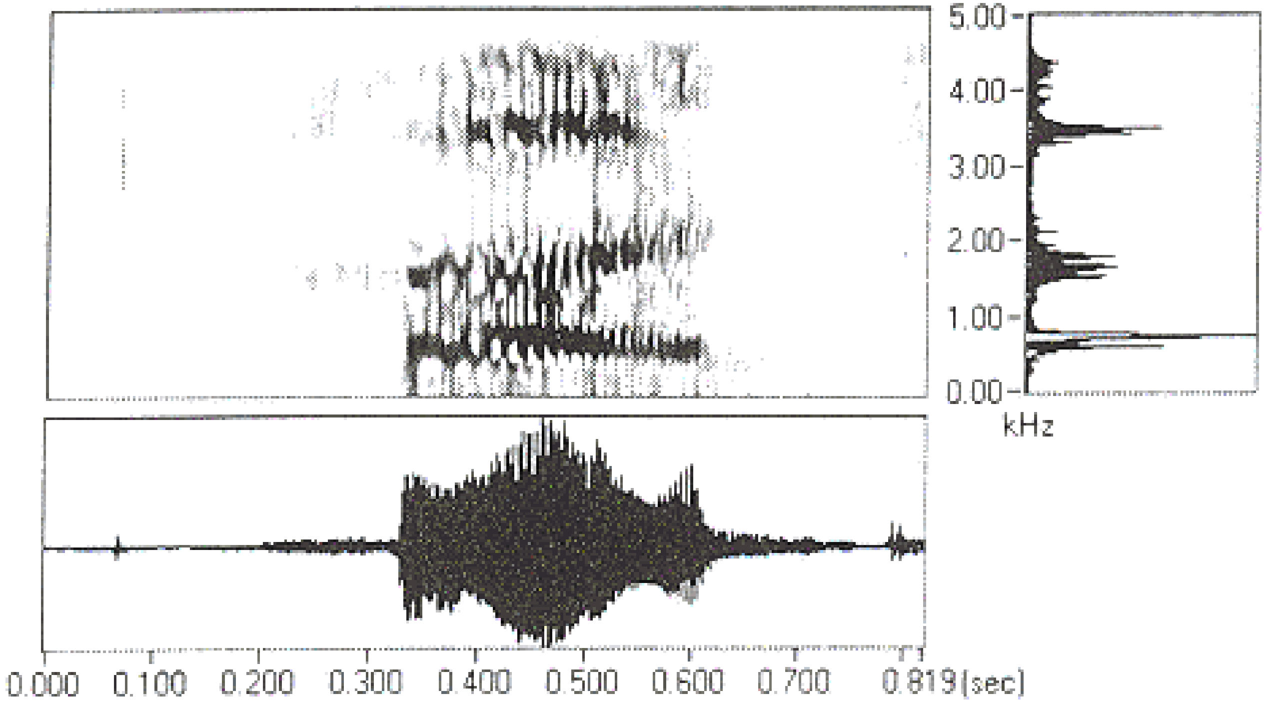
Re $\psi_{\ell m}(x)$

for l = 8 and m = 2



Izidor Gertner, City College, private comm.

$|F_{lm}(k)|$ for l = 8 and m = 2



The plot at the bottom of the figure is the time waveform of the word "hood" spoken by a five-year old boy.

The plot on the right is the standard power spectrum, which reveals four frequency tones.

The larger plot in the upper left is the time dependent spectrum, a function of both time and frequency

Summary:

1. The orthonormal set can be generalized for any real, square integrable function $\psi(x)$ of given parity [not just $\psi_o(x)$].
2. The set can be made double-peaked in *x* and shifted in *p.*
3. The set can be generalized to any dimension

- 4. GENERAL REMARK: In his book von Neumann wrote:

- ”We can prove the completeness of the resulting orthogonal set without particular difficulties… The proof of this fact leads to rather tedious calculations which require no new concepts, and we shall omit them.”

----Original message---
From Joshua Zak[mailto:zak@physics.technion.ac.il
Sent: Monday, July 28, 2003
To: bsimon@caltech.edu

Dear Barry,

As you requested I'm sending you the page from von Neumann's Book. Regards, Joshua

From: Barry Simon[mailto:bsimon@caltech.edu]
Sent: Tuesday, July 29, 2003

Dear Joshua,

I passed this on to a special functions expert that I know. I'll let you know
If he responds with anything useful. Barry

Bibliography: J.J. Halliwell, Phys.Rev. A72, 042109(2005)

$$\vec{R}_m = m_1\vec{a}_1 + m_2\vec{a}_2 \quad S = \left|\vec{a}_1 \times \vec{a}_2\right|$$

$$w_{\ell R_m}(\vec{r}) \equiv w_\ell(\vec{r} - \vec{R}_m)$$

$$\int w^*_{\ell R_m}(\vec{r}) w_{\ell' R_{m'}}(\vec{r}) d^2\vec{r} = \delta_{\ell\ell'}\delta_{R_m R_{m'}}$$

$$\psi_{\ell k}(\vec{r}) = \frac{S^{1/2}}{2\pi}\sum_{\vec{R}_m} \exp(i\vec{k}\vec{R}_m) w_\ell(\vec{r} - \vec{R}_m) = \frac{S^{1/2}}{2\pi}\sum_{\vec{R}_M} e^{i\vec{k}\vec{R}_m - \frac{i}{\hbar}\vec{p}\vec{R}_m} w_\ell(\vec{r})$$

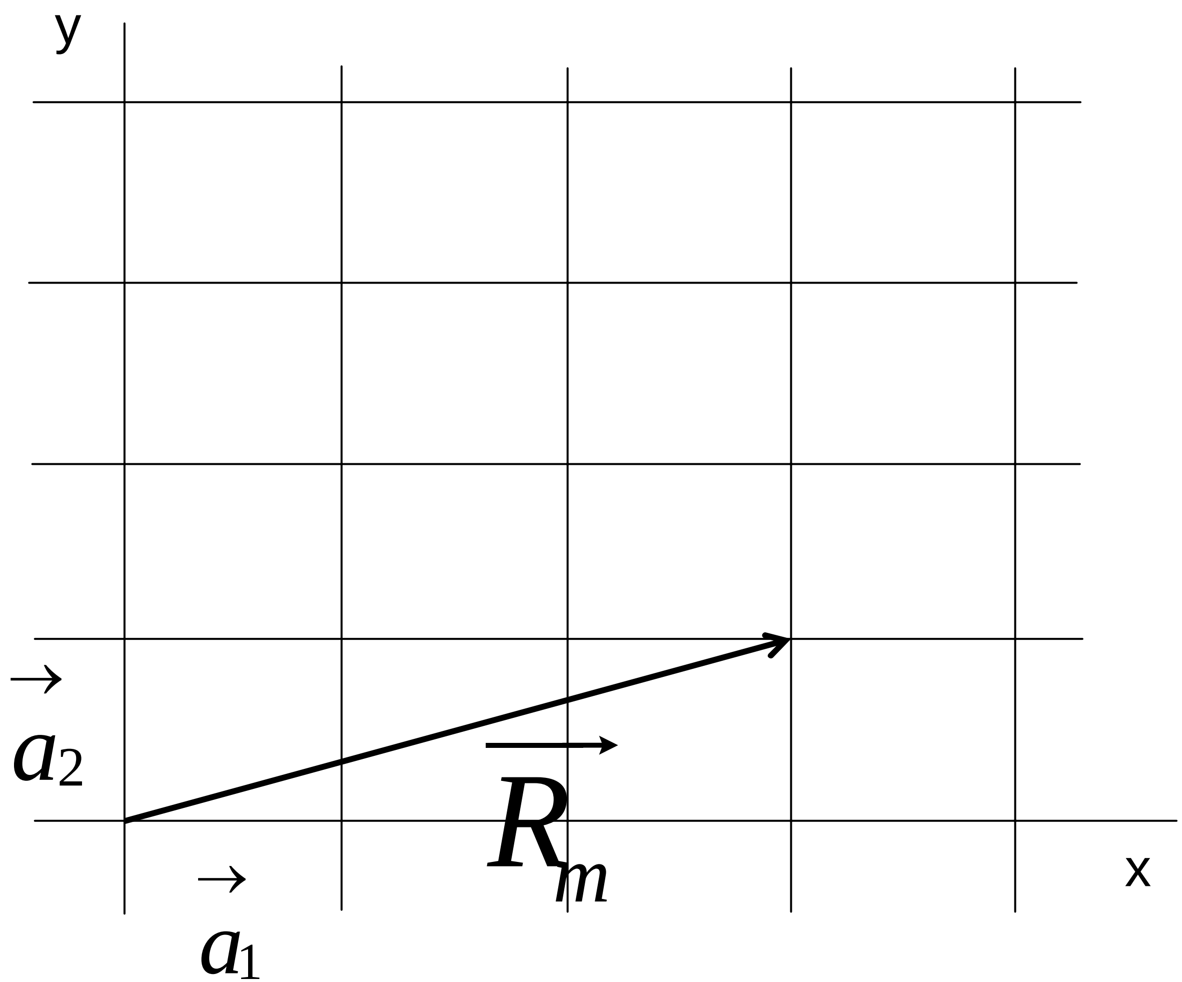
$$\vec{R}_m = m_1\vec{a}_1 + m_2\vec{a}_2 \quad S = \left|\vec{a}_1 \times \vec{a}_2\right|$$

$$w_{\ell R_m}(\vec{r}) \equiv w_\ell(\vec{r} - \vec{R}_m)$$

$$\int w^*_{\ell R_m}(\vec{r}) w_{\ell' R_{m'}}(\vec{r}) d^2\vec{r} = \delta_{\ell\ell'}\delta_{R_m R_{m'}}$$

$$\psi_{\ell k}(\vec{r}) = \frac{S^{1/2}}{2\pi}\sum_{\vec{R}_m}\exp(i\vec{k}\vec{R}_m) w_\ell(\vec{r} - \vec{R}_m) = \frac{S^{1/2}}{2\pi}\sum_{\vec{R}_M} e^{i\vec{k}\vec{R}_m - \frac{i}{\hbar}\vec{p}\vec{R}_m} w_\ell(\vec{r})$$

5.2 Two-dimensional crystal



5.4 Wannier Functions in a Magnetic Field

$$\psi_{\ell k}^{(m)}(\vec{r}) = \frac{S^{1/2}}{2\pi} \sum_{\vec{R}_m} e^{i\vec{k}\vec{R}_m} e^{-\frac{i}{\hbar}(\vec{p}-\frac{e}{2c}\vec{B}\times\vec{r})\vec{R}_m} w_\ell(\vec{r})$$

$$= \frac{S^{1/2}}{2\pi} \sum_{\vec{R}_m} e^{i\vec{k}\vec{R}_m + \frac{i}{\hbar}\frac{e}{2c}\vec{B}\times\vec{r}\vec{R}_m} w_\ell(\vec{r}-\vec{R}_m)$$

$e^{-\frac{i}{\hbar}(\vec{p}-\frac{e}{2c}\vec{B}\times\vec{r})\vec{R}_m} w_l(\vec{r})$: magnetic Wannier functions

$$e^{-\frac{i}{\hbar}(\vec{p}-\frac{e}{2c}\vec{B}\times\vec{r})\vec{R}_m} = e^{-\frac{i}{\hbar}\left(p_x+\frac{eB}{2c}y\right)m_1a_1-\frac{i}{\hbar}\left(p_y-\frac{eB}{2c}x\right)m_2a_2} =$$

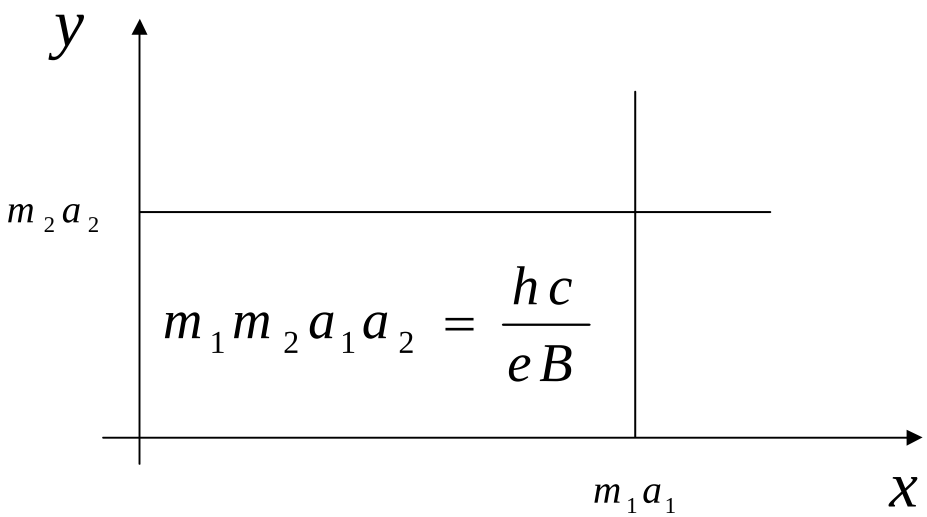
$$= e^{-\frac{im\omega}{\hbar}\left(\frac{1}{2}y+\frac{p_x}{m\omega}\right)m_1a_1+\frac{im\omega}{\hbar}\left(\frac{1}{2}x-\frac{p_y}{m\omega}\right)m_2a_2} =$$

$$= e^{-\frac{i}{\hbar}Pm_1a_1+\frac{im\omega}{\hbar}Xm_2a_2}$$

$$\psi_{\ell k}^{(m)}(\vec{r}) = \frac{S^{1/2}}{2\pi} \sum_{\vec{R}_m} e^{i\vec{k}\vec{R}_m} e^{-\frac{i}{\hbar}Pm_1 a_1 + \frac{i}{\hbar}m\omega X \;\; m_2 a_2} w_\ell(\vec{r})$$

Commuting Magnetic Translations

$$e^{-\frac{i}{\hbar} P\, m_1 a_1}\, e^{i\frac{m\omega}{\hbar} X\, m_2 a_2} = e^{i\frac{m\omega}{\hbar} X\, m_2 a_2}\, e^{-\frac{i}{\hbar} P\, m_1 a_1}\, e^{-i\hbar\, m_1 a_1 m_2 a_2 \frac{m\omega}{\hbar^2}}$$



Condition for the Magnetic Translations to commute