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On kq representations in quantum mechanics

R Jagannathan† and R Vasudevan‡

† Department of Physics, St Joseph's College, Tiruchirapalli 620 002, India
‡ Matscience, Institute of Mathematical Sciences, Madras 600 020, India

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Abstract. The Bloch-type functions for linear harmonic oscillators introduced recently by Krivoshlykov *et al* are shown to be identical to the kq representation functions of Zak. As a by-product of this analysis we obtain an interesting linear partial differential equation for Jacobi's θ_3 function with certain periodic boundary conditions. Finally we also point out briefly the relation between the so called coherent angular momentum states and kq-type representations.

1. Introduction

The main purpose of this paper is to analyse the relation between the kq representation functions of Zak (1967, 1968, 1972) and Bloch-type functions of a linear harmonic oscillator considered recently by Krivoshlykov *et al* (1977). Zak (1967) was the first to introduce the kq representation in quantum mechanics and demonstrate the convenience of using it in several problems of solid state physics (Zak 1972). Recently Krivoshlykov *et al* (1977) have introduced certain Bloch-type functions associated with any quantum system. They have also given the precise formulae expressing these Bloch-type functions through Jacobi's elliptic θ functions for several quantum systems. We shall call these Bloch-type functions of Krivoshlykov *et al* (1977) KMM Bloch functions. It is shown below that the normalised KMM Bloch functions for a linear harmonic oscillator constructed from its coherent states (Krivoshylkov *et al* 1977) are the same as Zak's kq representation functions.

2. Zak's functions and KMM Bloch functions

Following Zak (1972) let us define

$$\phi_{kq}(x; a) = (a/2\pi)^{1/2} \sum_{m=-\infty}^{\infty} \exp(\mathrm{i}kma)\delta(x+q-ma) \tag{2.1}$$

where $-\pi/a \leq k \leq \pi/a$ and $-\frac{1}{2}a \leq q \leq \frac{1}{2}a$. In order to make the comparison with KMM Bloch functions easier we have designated Zak's $\psi_{k,-q}(x; a)$ as $\phi_{kq}(x; a)$. Throughout the paper the δ functions such as $\delta(x+q-ma)$ in (2.1) refer to the familiar generalised functions called the Dirac delta functions (Dirac 1958). Since the $\{\phi_{kq}(x; a)\}$ are discrete sums of δ functions, they also belong to the class of generalised functions.

The kq representation functions $\{\phi_{kq}(x;a)\}$ defined by (2.1) form the set of basis functions for the one-dimensional representations of the Abelian group of operators

$$Z=\{\hat{Z}_{m_1m_2}=\exp(-\mathrm{i}m_1a\hat{p})\exp(\mathrm{i}2\pi m_2\hat{x}/a)|m_1, m_2=0, \pm 1, \pm 2, \ldots\} \tag{2.2}$$

with, as usual,

$$\hat{p}=-\mathrm{i}\partial/\partial x \qquad \hat{x}=x \qquad \hbar=1, \tag{2.3}$$

such that

$$\hat{Z}_{m_1m_2}\phi_{kq}(x;a)=\exp\{-\mathrm{i}[m_1ka+(2\pi m_2q/a)]\}\phi_{kq}(x;a). \tag{2.4}$$

As shown by Zak (1972), since $\{\phi_{kq}(x;a)\}$ are eigenfunctions of a complete set of commuting operators, they satisfy the orthogonality and closure relations

$$\langle kq|k'q'\rangle=\delta(k-k')\delta(q-q') \tag{2.5}$$

and

$$\int_{-a/2}^{a/2}\mathrm{d}q\int_{-\pi/a}^{\pi/a}\mathrm{d}k\langle x|kq\rangle\langle kq|x'\rangle=\delta(x-x') \tag{2.6}$$

respectively. The obvious three-dimensional generalisations of these kq representation functions have been established as very suitable basis functions in solid state problems where the parameters $\{a\}$ would be the appropriate lattice constants (Zak 1972).

Let us now define the projection operator (Wigner 1959) for the group Z, apart from the normalisation constant, as

$$\hat{P}_{kq}=\sum_{m_1,m_2=-\infty}^{\infty}\exp\{\mathrm{i}[km_1a+(2\pi m_2q/a)]\}\hat{Z}_{m_1m_2} \tag{2.7}$$

corresponding to the kqth representation

$$\Gamma_{kq}(\hat{Z}_{m_1m_2})=\exp\{-\mathrm{i}[km_1a+(2\pi m_2q/a)]\}. \tag{2.8}$$

Applying $\hat{P}$ on an arbitrary function $f(x)$ and using the identity

$$\sum_{m=-\infty}^{\infty}\exp[\mathrm{i}2\pi m(x+q)/a]=a\sum_{n=-\infty}^{\infty}\delta(x+q-na) \tag{2.9}$$

we find that

$$\begin{aligned}\hat{P}_{kq}f(x)&=\Big(\sum_{m_1=-\infty}^{\infty}\exp(\mathrm{i}km_1a)f(x-m_1a)\Big)\Big(\sum_{m_2=-\infty}^{\infty}\exp[\mathrm{i}2\pi m_2(x+q)/a]\Big)\\&=a\Big(\sum_{m_1=-\infty}^{\infty}\exp(\mathrm{i}km_1a)f(x-m_1a)\Big)\Big(\sum_{n=-\infty}^{\infty}\delta(x+q-na)\Big)\\&=a\Big(\sum_{l=-\infty}^{\infty}\exp(-\mathrm{i}kla)f(la-q)\Big)\Big(\sum_{n=-\infty}^{\infty}\exp(\mathrm{i}kna)\delta(x+q-na)\Big)\\&=a\Big(\sum_{l=-\infty}^{\infty}\exp(-\mathrm{i}kla)f(la-q)\Big)\phi_{kq}(x;a).\end{aligned} \tag{2.10}$$

Thus when any nonvanishing $\hat{P}_{kq}f(x)$ is normalised according to (2.5) one arrives at a unique $\phi_{kq}(x;a)$. This has to be so since the Abelian group of operators Z forms a complete set, as emphasised by Zak (1972). The Bloch-type nature of $\phi_{kq}(x; a)$ is evident from

$$\phi_{kq}(x+na; a)=\exp(\mathrm{i}kna)\phi_{kq}(x; a). \tag{2.11}$$

Let us now express the operator $\hat{Z}_{m_1m_2}$ of (2.2) in terms of the creation and annihilation operators of a linear harmonic oscillator of mass $m=1$ and circular frequency w. Then it is easy to see that

$$\hat{Z}_{m_1m_2}=(-1)^{m_1m_2}\exp(\alpha_{m_1m_2}b^{\dagger}-\alpha^*_{m_1m_2}b) \tag{2.12}$$

where

$$\begin{aligned} b &= (w^{1/2}\hat{x}+\mathrm{i}w^{-1/2}\hat{p})/\sqrt{2} \\ \alpha_{m_1m_2} &= (w^{1/2}q_0m_1+\mathrm{i}w^{-1/2}p_0m_2)/\sqrt{2} \\ q_0 &= a \qquad p_0=2\pi/a. \end{aligned} \tag{2.13}$$

In the notation of Krivoshlykov *et al* (1977)

$$\hat{Z}_{m_1m_2}=(-1)^{m_1m_2}D(\alpha_{m_1m_2})=\tilde{D}(\alpha_{m_1m_2}) \tag{2.14}$$

where the unitary operator $D(\alpha)$ is the well known coherent state generating operator. In terms of the expression (2.12) for $\hat{Z}_{m_1m_2}$ the projection operator $\hat{P}_{kq}$ of (2.7) reads

$$\hat{P}_{kq}=\sum_{m_1,m_2=-\infty}^{\infty}\exp[-\mathrm{i}(K_qm_1q_0+K_pm_2p_0)]^*\tilde{D}(\alpha_{m_1m_2}) \tag{2.15}$$

with a relabelling of k and q as K_q and K_p respectively. The expression on the right-hand side of (2.15) has been denoted as $\hat{V}_{K_qK_p}$ by Krivoshlykov *et al* (1977). Then, in view of (2.10) and (2.12)–(2.15), it is obvious that any normalised $\hat{V}_{K_qK_p}f(x)$ is given uniquely by $\phi_{K_qK_p}(x; q_0)$. In general, these $\hat{V}_{K_qK_p}f(x)$ have been called Bloch functions of the linear harmonic oscillator by Krivoshlykov *et al* (1977) since they obey

$$(\hat{V}_{K_qK_p}f)(x+nq_0)=\exp(\mathrm{i}K_qnq_0)(\hat{V}_{K_qK_p}f)(x) \tag{2.16}$$

as already pointed out in (2.11). In particular, they have taken $f(x)$ to be the coherent state

$$\langle x|\alpha\rangle=(w/\pi)^{1/4}\exp(-\tfrac{1}{2}\mathrm{i}wt)\exp\{-[(\tfrac{1}{2}w)^{1/2}x-\alpha]^2+\tfrac{1}{2}(\alpha^2-|\alpha|^2)\} \tag{2.17}$$

with α as any complex number and have shown that

$$\begin{aligned} \hat{V}_{K_qK_p}\langle x|\alpha\rangle &= \langle x|\alpha; K_q, K_p\rangle \\ &= \langle x|\alpha\rangle\theta_3[1|p_0(x+K_p)]/2\pi \\ &\quad\times\theta_3(\exp(-\tfrac{1}{2}q_0{}^2w)|q_0[K_q+\mathrm{i}(2w)^{1/2}\alpha-\mathrm{i}wx]/2\pi) \end{aligned} \tag{2.18}$$

where

$$\theta_3(u|v)=\sum_{m=-\infty}^{\infty}u^{m^2}\exp(\mathrm{i}2\pi mv) \tag{2.19}$$

defines the Jacobi θ_3 function (Jeffreys and Jeffreys 1962).

It has been claimed (Krivoshlykov *et al* 1977) that where coherent states have been useful the above Bloch-type functions (2.18) can be used. As we have shown above, when suitably normalised the above so called oscillator Bloch functions become just

$\{\phi_{K_qK_p}(x;q_0)\}$ or Zak's $\{\psi_{K_q,-K_p}(x;q_0)\}$. The above form of (2.18) can be understood easily if we recognise that (2.10) can be written equivalently as

$$\hat{P}_{Kq}f(x)=\left(\sum_{m=-\infty}^{\infty}\exp(ikma)f(x-ma)\right)\theta_3(1|(x+q)/a) \tag{2.20}$$

when we write formally

$$\sum_{m=-\infty}^{\infty}\exp[i2\pi(x+q)/a]=\theta_3(1|(x+q)/a) \tag{2.21}$$

as done by Krivoshlykov *et al* (1977) in deriving (2.18).

It is evident that the set $\{\langle x|\alpha;K_q,K_p\rangle|-\pi/q_0\leqslant K_q\leqslant\pi/q_0,\ -\pi/p_0\leqslant K_p\leqslant\pi/p_0\}$ is complete since they are identical with the set of $\phi_{K_qK_p}(x;q_0)$ functions obeying (2.6). When (q_0,p_0) in (2.13) are chosen such that $q_0p_0=2\pi n$, with $n>1$ this completeness would be lost since the set $\{\tilde{D}(\alpha_{m_1m_2})|m_1,m_2=0,\pm1,\pm2,\dots\}$ does not contain all the elements of the complete set of commuting operators $\{\hat{Z}_{m_1m_2}|m_1,m_2=0,\pm1,\pm2,\dots\}$ of (2.2). The same conclusion on the completeness of the set of functions $\{\langle x|\alpha;K_q,K_p\rangle\}$ has been reached by Krivoshlykov *et al* (1977) quite differently.

3. Jacobi's θ_3 functions

The above analysis leads to the following interesting result regarding Jacobi's θ_3 function. When any function $f(x)$ is expressed in terms of Zak's functions

$$\begin{aligned}\psi_{kq}(x;a)&=\phi_{k,-q}(x;a)\\&=(a/2\pi)^{1/2}\sum_{m=-\infty}^{\infty}\exp(ikma)\delta(x-q-ma)\end{aligned} \tag{3.1}$$

as

$$f(x)=\int_{-\pi/a}^{\pi/a}dk\int_{-a/2}^{a/2}dq\langle kq|f\rangle\psi_{kq}(x;a) \tag{3.2}$$

the expansion coefficients

$$\langle kq|f\rangle=(a/2\pi)^{1/2}\sum_{m=-\infty}^{\infty}\exp(-ikma)f(q+ma) \tag{3.3}$$

obey the Bloch property (Zak 1972)

$$\langle k+(2\pi r/a),q+na|f\rangle=\exp(ikna)\langle kq|f\rangle \qquad r,n=0,\pm1,\pm2,\dots. \tag{3.4}$$

In the kq representation with $\{\psi_{kq}(x;a)\}$ as basis the operators $\{\hat{x},\hat{p}\}$ become (Zak 1972)

$$\hat{x}=i(\partial/\partial k)+\hat{q} \qquad \hat{p}=-i(\partial/\partial q). \tag{3.5}$$

Let $f(x)$ be a solution of a linear differential equation

$$L(\hat{x},\hat{p})f(x)=0. \tag{3.6}$$

Then obviously $\langle kq|f\rangle$ given by (3.3) must be a solution of the differential equation

$$L((i\partial/\partial k)+\hat{q},\ -i\,\partial/\partial q)C(kq)=0 \tag{3.7}$$

along with the periodicity conditions of (3.4). We shall consider a simple example below. We know very well from the study of the quantum harmonic oscillator that

$$(\hat{x}+\mathrm{i}\hat{p})f(x)=0 \tag{3.8}$$

has the solution

$$f(x)=\exp(-\tfrac{1}{2}x^2). \tag{3.9}$$

In the kq representation (3.8) becomes

$$[(\mathrm{i}\partial/\partial k)+q+(\partial/\partial q)]\langle kq|f\rangle=0 \tag{3.10}$$

where the appropriate solution $\langle kq|f\rangle$ obeying (3.4) is found to be

$$\begin{aligned}\langle kq|f\rangle&=\langle kq|\exp(-\tfrac{1}{2}x^2)\rangle\\&=(a/2\pi)^{1/2}\exp(-\tfrac{1}{2}q^2)\theta_3[\exp(-\tfrac{1}{2}a^2)|a(k-\mathrm{i}q)/2\pi]\end{aligned} \tag{3.11}$$

using (2.19) and (3.3). Now substituting (3.11) in (3.10) we get

$$[(\mathrm{i}\partial/\partial k)+(\partial/\partial q)]\theta_3(\exp(-\tfrac{1}{2}a^2)|a(k-\mathrm{i}q)/2\pi)=0. \tag{3.12}$$

Thus we realise the interesting fact that $\theta_3(\exp(-\frac{1}{2}a^2)|a(k-\mathrm{i}q)/2\pi)$ is a solution of

$$[(\mathrm{i}\partial/\partial k)+(\partial/\partial q)]C(kq)=0 \tag{3.13}$$

subject to the periodic boundary conditions

$$\begin{aligned}&\exp[-\tfrac{1}{2}(q+na)^2]C(k+(2\pi r/a),(q+na))\\&\quad=\exp[\mathrm{i}kna-(\tfrac{1}{2}q^2)]C(kq)\qquad r,n=0,\pm1,\pm2,\ldots\end{aligned} \tag{3.14}$$

obtained from (3.4) and (3.11). One can also see directly that (3.13) and (3.14) lead to (3.12) as follows. Applying the method of separation of variables to (3.13) and requiring the general solution to obey (3.14), corresponding to the case $n=0$, $r=\pm1$, $\pm2,\ldots$, we get

$$C(kq)=\sum_{s=-\infty}^{\infty}F(sa)\exp[\mathrm{i}sa(k-\mathrm{i}q)] \tag{3.15}$$

where the $F(sa)$ are constants. Further use of (3.14) for the case $r=0$, $m=\pm1,\pm2,\ldots$ leads to the recurrence relation

$$F((s+t)a)=F(sa)\exp[-\tfrac{1}{2}a^2(t^2+2st)]\qquad s,t=0,\pm1,\pm2,\ldots, \tag{3.16}$$

showing that

$$F(sa)=\exp(-\tfrac{1}{2}s^2a^2)F(0)\qquad s=0,\pm1,\pm2,\ldots. \tag{3.17}$$

Then on taking $F(0)=1$, (3.15) becomes

$$\begin{aligned}C(kq)&=\sum_{s=-\infty}^{\infty}\exp(-\tfrac{1}{2}s^2a^2)\exp[\mathrm{i}sa(k-\mathrm{i}q)]\\&=\theta_3(\exp(-\tfrac{1}{2}a^2)|a(k-\mathrm{i}q)/2\pi),\end{aligned} \tag{3.18}$$

consistent with (3.12).

4. On angular momentum coherent states

In conclusion, let us also make the following observation. In quantum mechanics describing $(\hat{J}_z, \hat{\varphi})$ and similar number and phase operators as canonically conjugate has presented well known difficulties (Sussikind and Glogower 1964, Carruthers and Nieto 1968). Here, since the angular coordinate is confined to the range $(0, 2\pi)$, the kq representation as suggested by Zak (1969) is the natural choice. The eigenstates in this case correspond to the set of commuting operators generated by $\exp(i2\pi\hat{J}_z)$ and $\exp(i\hat{\varphi})$. Hence the kq representation yields for the eigenstates of $\exp(i\hat{\varphi})$

$$\begin{aligned}\psi_{\varphi'}(\varphi) &= \sum_{m=-\infty}^{\infty} \delta(\varphi - \varphi' - 2m\pi) \\ &= (1/2\pi) \sum_{m=-\infty}^{\infty} \exp[i(\varphi - \varphi')m] \end{aligned} \tag{4.1}$$

since $\hat{J}_z$ has only integer eigenvalues (Zak 1969). Recently (Levy Leblond 1973, Santhanam 1977), starting with angular momentum states $|j, m\rangle$, diagonal in $\hat{J}_z$, states diagonal in $\exp(i\hat{\varphi})$ have been obtained. Santhanam (1977) has obtained states such as

$$|j, \mu = \exp(i\varphi)\rangle \sim \sum_{m=-j}^{j} \exp[-i2\pi\mu(m + j\hat{I})/(2j+1)]|j, m\rangle \tag{4.2}$$

where $\hat{I}$ is the identity operator. Taking the limit $j \to \infty$ it can be shown (Santhanam and Vasudevan 1978) that (4.2) leads to the result that

$$\langle\varphi|\varphi'\rangle \sim \sum_{m=-\infty}^{\infty} \exp[-im(\varphi' - \varphi)] \tag{4.3}$$

is diagonal in $\exp(i\hat{\varphi})$ as seen already in (4.1). Even though the finite j states $\{|j, \mu\rangle\}$ of (4.2) have been called angular momentum coherent states in the papers cited above, the corresponding uncertainty products do not turn out to be minimum. Actually, as pointed out by Zak (1972), the kq representations belong to the situation in which the uncertainty products will rather be maximum.

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References

Carruthers P and Nieto M M 1968 *Rev. Mod. Phys.* **40** 411
Dirac P A M 1958 *The Principles of Quantum Mechanics* 4th edn (London: Oxford University Press) ch III
Jeffreys H and Jeffreys B S 1962 *Methods of Mathematical Physics* 3rd edn (London: Cambridge University Press) ch 25
Krivoshlykov S G, Malkin I A and Man'ko V I 1977 *P N Lebedev Physical Institute, Moscow Preprint No 25*
Levy Leblond J M 1973 *Rev. Mex. Fis.* **22** 15
Santhanam T S 1977 *Foundations of Physics* **7** 191
Santhanan T S and Vasudevan R 1978 *Institute of Mathematical Sciences, Madras Preprint*
Sussikind L and Glogower J 1964 *Physica* **1** 49

Wigner E P 1959 *Group Theory and its Applications to Quantum Mechanics of Atomic Spectra* (New York: Academic) ch 12
Zak J 1967 *Phys. Rev. Lett.* **19** 1385
—— 1968 *Phys. Rev.* **168** 686
—— 1969 *Phys. Rev.* **187** 1803
—— 1972 *Solid St. Phys.* **27** 1