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Crystal electrons in magnetic fields: General reduction of the dimensionality and properties of the wave functions

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The motion of Bloch electrons in homogeneous magnetic fields is reduced without approximations to, at most, two dimensions in the general three-dimensional case, i.e., for arbitrary crystal potential, arbitrary field-lattice geometry, and all rational fields. This is done by fully exploiting a canonical transformation and by constructing with the aid of ray-group projection operators generalized k-q functions, which separate off one degree of freedom. Previous *ad hoc* reductions to one dimension for essentially two-dimensional situations are recovered and explained. The solutions of the resulting lower-dimensional effective Schrödinger equations are functions of generalized coordinates. They are converted into the real-space wave functions by means of a contact transformation; their local and global properties are investigated. The results presented allow first-principles calculations of diamagnetic band structures and wave functions to realistic systems.

I. INTRODUCTION

In recent years methods have been developed[1–4] which allow calculations from first principles and to high precision the energy spectrum and the wave functions of crystal electrons in a homogeneous magnetic field. One of the concepts involved is the reduction of the problem to a one-dimensional problem by means of a canonical transformation and a special separation ansatz. A different reduction procedure has been derived independently by Wannier.[5]

Both these reduction methods apply only to essentially two-dimensional systems: In Refs. 1–4 the assumption is made from the outset that the motion of the charged particle along the magnetic field completely decouples from that within the plane normal to the field. Wannier's approach, on the other hand, requires the influence of the variation of the crystal potential along the field to vanish altogether. Therefore, as can be shown easily, his treatment of "triclinic" lattices is equivalent to the treatment of monoclinic crystals presented in Refs. 1–3.

Some years ago Zak[6] had already worked out the reduction to one dimension for two-dimensional lattices and very special magnetic fields perpendicular to the lattice plane.

In almost all realistic situations all those restrictive conditions for the field-lattice geometry and the periodic potential are not met; thus nearly always one has to deal with a genuine three-dimensional situation. This is certainly true for all real crystals and even for such an artificial system as a two-dimensional lattice with the magnetic field pointing in any direction except perpendicular or parallel to the lattice plane normal.

In the first part of this paper (Secs. II and III) it will be shown how the reduction of the dimensionality of the problem can be achieved for arbitrary periodic potential and general rational field by constructing equivalent, at most two-dimensional Hamiltonians. This construction takes full advantage of two main concepts: (i) the theory of the magnetic translation group along the lines marked by Brown and Fischbeck (see, for example, Refs. 7 and 8) and (ii) the canonical transformation introduced in Refs. 1–3. Owing to the combination of both tools the reduction procedure becomes very simple and perfectly straightforward. The *ad hoc* techniques used in Refs. 1–3 and 5 can be explained as special cases of the general approach, which, as a secondary effect, also produces all quantum numbers of the problem.

In the second part (Sec. IV) the mathematical structure and the physical properties of the di-

amagnetic wave functions will be investigated. This analysis is based on the results obtained in Sec. III and in previous model calculations[2,4] for the "equivalent" solutions, i.e., for the stationary states as functions of the generalized coordinates. As a prerequisite, concise transformation formulas will be derived, which allow us to find in a simple way the "true" wave functions from the equivalent ones and vice versa.

II. TRANSFORMATION OF THE OPERATORS

The Hamiltonian for an electron in a periodic potential and a magnetic field is

$$\mathcal{H}=\frac{1}{2m}\left[\vec{p}-\frac{e}{c}\vec{A}(\vec{r})\right]^2+V(\vec{r}) , \tag{2.1}$$

where $V(\vec{r}+\vec{R})=V(\vec{r})$ for all lattice vectors $\vec{R}$ and $\vec{A}$ is the vector potential. Denoting the primitive vectors of the lattice by $\vec{a}_1$, $\vec{a}_2$, and $\vec{a}_3$, we have

$$\vec{R}=\sum_{i=1}^{3} n_i\vec{a}_i, \quad n_i\in\mathcal{Z} . \tag{2.2}$$

The primitive vectors of the reciprocal lattice $\vec{b}_1,\vec{b}_2,\vec{b}_3$ and the general reciprocal-lattice vector $\vec{G}$ are then defined by

$$\begin{aligned}&\vec{a}_i\cdot\vec{b}_j=\delta_{ij},\\ &\vec{G}=2\pi\sum_{i=1}^{3} g_i\vec{b}_i, \quad g_i\in\mathcal{Z} .\end{aligned} \tag{2.3}$$

We will consider general rational magnetic fields (in the sense of Brown and Fischbeck[7,8]) which form a dense subset of the set of all possible magnetic fields. Without loss of generality we choose $\vec{B}\|\vec{a}_3$. Then

$$\frac{e\vec{B}}{\hbar c}=\frac{2\pi}{\Omega}\frac{L}{N}\vec{a}_3 , \tag{2.4}$$

where L and N are integers without common factor and $\Omega=(\vec{a}_1\times\vec{a}_2)\cdot\vec{a}_3$.

In view of the reduction procedure below there is an optimal choice of the Cartesian system of axes.[9] Let

$$\hat{z}\equiv\frac{\vec{a}_3}{|\vec{a}_3|} , \tag{2.5}$$

implying $\vec{B}\equiv B\hat{z}$. Defining $\alpha\equiv eB/\hbar c$ and $\vec{\alpha}\equiv\alpha\hat{z}$ all rational magnitudes of the field are given by

$$\alpha=\frac{2\pi}{\Omega}\frac{L}{N}|\vec{a}_3| . \tag{2.6}$$

Because of Eq. (2.3) we are free to choose

$$\hat{x}\equiv\frac{\vec{b}_1}{|\vec{b}_1|} . \tag{2.7}$$

Introducing the notation $a_1^x\equiv\vec{a}_1\cdot\hat{x}$, $b_1^x\equiv\vec{b}_1\cdot\hat{x}$, etc. we then get

$$\begin{aligned}&a_2^x=0, \quad |\vec{b}_1|=b_1^x, \quad |\vec{a}_3|=a_3^z ,\\ &a_1^x=1/b_1^x, \quad b_3^z=1/a_3^z ,\end{aligned} \tag{2.8a}$$

$$\Omega=a_1^x a_2^y a_3^z , \tag{2.8b}$$

$$\alpha=\frac{2\pi}{a_1^x a_2^y}\frac{L}{N} . \tag{2.8c}$$

Without exception we will use the symmetrical gauge for $\vec{A}$, i.e.,

$$\vec{A}=\tfrac{1}{2}\vec{B}\times\vec{r}=\frac{B}{2}(-y\hat{x}+x\hat{y}) . \tag{2.9}$$

Now Eq. (2.1) may be written as[1-3]

$$\mathcal{H}=\frac{\hbar\omega_c}{2}\left[\left[\frac{\alpha^{1/2}}{2}y+\frac{\alpha^{-1/2}}{\hbar}p_x\right]^2+\left[\frac{\alpha^{1/2}}{2}x-\frac{\alpha^{-1/2}}{\hbar}p_y\right]^2\right]+\frac{p_z^2}{2m}+\sum_{\vec{G}} v(\vec{G})\exp[i\vec{G}\cdot(x\hat{x}+y\hat{y}+z\hat{z})] , \tag{2.10}$$

where we have Fourier-expanded $V(\vec{r})$ and defined $\omega_c\equiv eB/mc$.

The magnetic translation operators, which form a ray group[7,8] when $\vec{R}$ runs through the lattice, are given by

$$\begin{aligned}T_M(\vec{R})&=\exp\left[\frac{i}{\hbar}\vec{R}\cdot\left[\vec{p}+\frac{e}{c}\vec{A}\right]\right]\\ &=\exp\left\{i\alpha^{1/2}\vec{R}\left[\left[-\frac{\alpha^{1/2}}{2}y+\frac{\alpha^{-1/2}}{\hbar}p_x\right]\hat{x}+\left[\frac{\alpha^{1/2}}{2}x+\frac{\alpha^{-1/2}}{\hbar}p_y\right]\hat{y}+\left[\frac{\alpha^{-1/2}}{\hbar}p_z\right]\hat{z}\right]\right\} .\end{aligned} \tag{2.11}$$

Of course we have

$$[\mathscr{H},T_M(\vec{\mathrm{R}})]=0\ , \tag{2.12a}$$

$$T_M(\vec{\mathrm{R}})T_M(\vec{\mathrm{R}}')=\exp\left[\frac{i}{2}(\vec{\mathrm{R}}\times\vec{\mathrm{R}}')\vec{\alpha}\right]T(\vec{\mathrm{R}}+\vec{\mathrm{R}}') \tag{2.12b}$$

for all $\vec{\mathrm{R}},\vec{\mathrm{R}}'$. We now introduce generalized coordinate and momentum operators (see also Refs. 1–3):

$$\begin{aligned}&\tilde{x}=\frac{\alpha^{1/2}}{2}x-\frac{\alpha^{-1/2}}{\hbar}p_y,\ \ \tilde{y}=\frac{\alpha^{1/2}}{2}x+\frac{\alpha^{-1/2}}{\hbar}p_y,\ \ \tilde{z}=\alpha^{1/2}z\ ,\\ &\tilde{p}_x=\frac{\alpha^{1/2}}{2}y+\frac{\alpha^{-1/2}}{\hbar}p_x,\ \ \tilde{p}_y=-\frac{\alpha^{1/2}}{2}y+\frac{\alpha^{-1/2}}{\hbar}p_x,\ \ \tilde{p}_z=\frac{\alpha^{-1/2}}{\hbar}p_z\ ,\end{aligned} \tag{2.13a}$$

implying

$$\begin{aligned}&x=\alpha^{-1/2}(\tilde{x}+\tilde{y}),\ \ y=\alpha^{-1/2}(\tilde{p}_x-\tilde{p}_y),\ \ z=\alpha^{-1/2}\tilde{z}\ ,\\ &p_x=\frac{\hbar}{2}\alpha^{1/2}(\tilde{p}_x+\tilde{p}_y),\ \ p_y=\frac{\hbar}{2}\alpha^{1/2}(-\tilde{x}+\tilde{y}),\ \ p_z=\hbar\alpha^{1/2}\tilde{p}_z\ .\end{aligned} \tag{2.13b}$$

The new observables are canonically conjugated:

$$[\tilde{x},\tilde{p}_x]=[\tilde{y},\ \tilde{p}_y]=[\tilde{z},\ \tilde{p}_z]=i\ . \tag{2.14}$$

All other commutators vanish.

In rotated phase space the Hamiltonian assumes the form

$$\tilde{\mathscr{H}}=\frac{\hbar\omega_c}{2}(\tilde{p}_x^2+\tilde{x}^2)+\frac{\hbar\omega_c}{2}\tilde{p}_z^2+\sum_{\vec{\mathrm{G}}}v(\vec{\mathrm{G}})\exp\{\,i\alpha^{-1/2}\vec{\mathrm{G}}\cdot[(\tilde{x}+\tilde{y})\hat{x}+(\tilde{p}_x-\tilde{p}_y)\hat{y}+\tilde{z}\hat{z}]\,\}\ . \tag{2.15}$$

The Fourier components of the periodic potential will be factorized as follows:

$$\begin{aligned}V(\vec{\mathrm{G}};\tilde{x},\tilde{y},\tilde{z})&\equiv v(\vec{\mathrm{G}})\exp\{\,i\alpha^{-1/2}\vec{\mathrm{G}}\cdot[(\tilde{x}+\tilde{y})\hat{x}+(\tilde{p}_x-\tilde{p}_y)\hat{y}+\tilde{z}\hat{z}]\,\}\\ &=v(\vec{\mathrm{G}})X(\vec{\mathrm{G}};\tilde{x},\tilde{p}_x)Y(\vec{\mathrm{G}};\tilde{y},\tilde{p}_y)Z(g_3;\tilde{z})\ ,\end{aligned} \tag{2.16}$$

with

$$\begin{aligned}&X(\vec{\mathrm{G}};\tilde{x},\tilde{p}_x)\equiv\exp[i\alpha^{-1/2}\vec{\mathrm{G}}\cdot(\tilde{x}\hat{x}+\tilde{p}_x\hat{y})]\ ,\\ &Y(\vec{\mathrm{G}};\tilde{y},\tilde{p}_y)\equiv\exp[i\alpha^{-1/2}\vec{\mathrm{G}}\cdot(\tilde{y}\hat{x}-\tilde{p}_y\hat{y})]\ ,\\ &Z(g_3i\tilde{z})\equiv\exp\left[i\frac{2\pi}{\alpha^{1/2}}b_3^z g_3\tilde{z}\right]\ .\end{aligned} \tag{2.17}$$

For the magnetic translation operators we get

$$\tilde{T}_M(\vec{\mathrm{R}})=\exp[i\alpha^{1/2}\vec{\mathrm{R}}\cdot(\tilde{p}_y\hat{x}+\tilde{y}\hat{y}+\tilde{p}_z\hat{z})]\ . \tag{2.18}$$

Note that we have achieved through the canonical transformation (2.13) a simultaneous reduction of the originally three-dimensional magnetic translation "group" and of the kinetic part of the Hamiltonian to two degrees of freedom.

III. REDUCTION OF THE DIMENSIONALITY

The new observables (2.13a) belong to a pseudosystem with three degrees of freedom.

Throughout this section we exclusively refer to this system and therefore drop the tildes: $\tilde{x}\to x$, etc. Choosing the coordinate representation all operators act on a vector space of functions $f(x,y,z)$. This space, which will be called $S(\mathscr{R}^3)$, is spanned by the simultaneous eigenfunctions of the commutating new coodinate operators, i.e., by the product basis

$$\{\,\delta(x-x_0)\delta(y-y_0)\delta(z-z_0)\,|\,x_0,y_0,z_0\in\mathscr{R}\,\}\ .$$

In other words,

$$S(\mathscr{R}^3)=S(\mathscr{R}_x)\times S(\mathscr{R}_y)\times S(\mathscr{R}_z)\ ,$$

where $S(\mathscr{R}_x)$ denotes the function space associated with the x degree of freedom, etc. Equation (2.14) of course implies

$$p_x=\frac{1}{i}\frac{\partial}{\partial x},\ \ p_y=\frac{1}{i}\frac{\partial}{\partial y},\ \ p_z=\frac{1}{i}\frac{\partial}{\partial z}\ . \tag{3.1}$$

Now, quite analogous to the normal case of an "ordinary" symmetry group, the Hamiltonian (2.15) does not couple functions out of $S(\mathscr{R}^3)$,

which belong to different irreducible ray representations[7,8] of the magnetic translation "group" (2.18) or to different rows of the same irreducible ray representation. Owing to this fact the eigenvalue problem associated with $\mathscr{H}$ can be greatly simplified by decomposing $S(\mathscr{R}^3)$ into invariant subspaces with the aid of ray-group projection operators.

Now it is a decisive advantage that after the canonical transformation (2.13) has been performed the full ray group of magnetic translations does not act on $S(\mathscr{R}^3)$ but only on the smaller function space $S(\mathscr{R}_y)\times S(\mathscr{R}_z)$. It therefore becomes "too large" and, as a consequence, the decomposition into invariant subspaces will be so effective that the y dependence of the wave functions can be projected out completely. This is demonstrated below.

For a general rational field as given by Eq. (2.4) the magnetic translation group has the following nonequivalent unitary irreducible ray representations (see also Refs. 7 and 8):

$$D^{\vec{q}}(\vec{R})=\exp(i\vec{q}\cdot\vec{R})D^0(\vec{R})\ , \tag{3.2}$$

where

$$D^0_{tt'}(\vec{R})=\exp\left[i\pi\frac{L}{N}n_1[n_2+2(t'-1)]\right]\delta_{t,t'+n_2}(\mathrm{mod}N),\quad t,t'=1,2,\ldots,N \tag{3.3}$$

and $\vec{q}$ spans the magnetic Brillouin zone:

$$\vec{q}=q_1\vec{b}_1+q_2\vec{b}_2+q_3\vec{b}_3,\quad q_1,q_2\in\left[0,\frac{2\pi}{N}\right],\quad q_3\in[0,2\pi)\ . \tag{3.4}$$

We will now decompose an appropriate basis of $S(\mathscr{R}_y)\times S(\mathscr{R}_z)$ into sets of N functions each, which transform identically according to $D^{\vec{q}}$ when the operators $T_M(\vec{R})$ act upon them. Then, if $f^{\vec{q}}(t,m;y,z)$ denotes the tth partner of the mth set, the set of symmetry-adapted functions

$$\{f^{\vec{q}}(t,m;y,z)\,|\,m=1,2,\ldots;\ t,\vec{q}\ \text{fixed}\}$$

spans an invariant subspace with respect to $\mathscr{H}$.

The decomposition is achieved by means of the ray-group projection operators

$$P^{\vec{q}}_{11}=\sum_{\vec{R}}\{D^{\vec{q}}_{11}(\vec{R})\}^*T_M(\vec{R})\ , \tag{3.5}$$

which yield the first partner, and the simple relation[7]

$$f^{\vec{q}}(t,m)=\exp[-iq_2(t-1)]T_M((t-1)\vec{a}_2)f^{\vec{q}}(1,m)\ . \tag{3.6}$$

Using (2.8c) and (2.12b) we easily find

$$T_M(\vec{R})=\exp\left[-i\pi\frac{L}{N}n_1n_2\right]\left[\exp\left[-i\frac{\alpha}{2}a_1^xa_1^yn_1^2\right]T_y(\alpha^{1/2}a_1^xn_1)\exp(i\alpha^{1/2}a_1^yn_1y)T_z(\alpha^{1/2}a_1^zn_1)\right]$$
$$\times[\exp(i\alpha^{1/2}a_2^yn_2y)T_z(\alpha^{1/2}a_2^zn_2)][T_z(\alpha^{1/2}a_3^zn_3)]\ , \tag{3.7}$$

where T_y and T_z denote ordinary translation operators:

$$T_y(c)g(y,z)=g(y+c,z)\quad\text{and}\quad T_z(d)g(y,z)=g(y,z+d)\ .$$

From Eqs. (3.3), (3.5), and (3.7) we immediately find

$$P^{\vec{q}}_{11}=\left[\sum_{n_1\in\mathscr{Z}}\exp(-iq_1n_1)\exp\left[-i\frac{\alpha}{2}a_1^xa_1^yn_1^2\right]T_y(\alpha^{1/2}a_1^xn_1)\exp(i\alpha^{1/2}a_1^yn_1y)T_z(\alpha^{1/2}a_1^zn_1)\right]$$
$$\times\left[\sum_{r\in\mathscr{Z}}\exp(-iq_2Nr)\exp(i\alpha^{1/2}a_2^yNry)T_z(\alpha^{1/2}a_2^zNr)\right]\times\left[\sum_{n_3\in\mathscr{Z}}\exp(-iq_3n_3)T_z(\alpha^{1/2}a_3^zn_3)\right]\ , \tag{3.8}$$

where r is a new index entering through n_2 and the summations are completely decoupled.

As can be directly seen from Eqs. (3.2) and (3.3) the symmetry-adapted functions must behave as Bloch-type functions under the action of the operators $T_M(n_3\vec{a}_3)$ (which together form an Abelian subgroup of the magnetic translation group), i.e.,

$$T_M(n_3\vec{a}_3)f^{\vec{q}}(t,m)=\exp(iq_3n_3)f^{\vec{q}}(t,m)\ . \tag{3.9}$$

Hence we choose for $S(\mathscr{R}_y)\times S(\mathscr{R}_z)$ the pre-adapted basis

$$b(q_3,s,y_0;y,z)\equiv\exp\left[i\frac{b_3^z}{\alpha^{1/2}}(q_3+2\pi s)z\right]\delta(y-y_0),\quad s\in\mathscr{Z},\quad y_0\in\mathscr{R}\ . \tag{3.10}$$

In the following we will distinguish two cases.

A. $\vec{a}_1,\vec{a}_2\perp\vec{a}_3$

We begin by considering the very special situation when $\vec{a}_1$ and $\vec{a}_2$ simultaneously are perpendicular to $\vec{a}_3$ and therefore to $\vec{B}$. The treatment of this simpler case will feature the reduction method and recover all results from previous work[1,3,5,6] in an easy and systematic way.

In addition to Eq. (2.8a) we now have $a_1^z=a_2^z=0$. Using this the decomposition of the basis (3.10) into irreducible function sets by means of the projection operators (3.8) and the relation (3.6) becomes a rather simple procedure. We find that the different sets transforming according to a certain $D^{\vec{q}}$ can be classified by the indices $l=1,2,\ldots,L$ and $s\in\mathscr{Z}$. The tth partner $\phi^{\vec{q}}(t,s,l)$ of such a set is given by

$$\begin{aligned}\phi^{\vec{q}}(t,s,l;y,z)=\exp\left[i\frac{b_3^z}{\alpha^{1/2}}(q_3+2\pi s)z\right]\sum_{m\in\mathscr{Z}}\exp\left[i\frac{2\pi}{N}(t-1)(l+Lm)\right]\exp\left[i\left[q_1-\frac{a_1^y}{a_2^y}q_2\right]m\right]\\ \times\exp\left[-i\frac{\alpha}{2}a_1^xa_1^y\left[m^2+\frac{2l}{L}m\right]\right]\\ \times\delta\left[y-\alpha^{1/2}a_1^xm-\alpha^{1/2}a_1^x\frac{l}{L}-\frac{\alpha^{1/2}}{2\pi}a_1^x\frac{N}{L}q_2\right].\end{aligned} \tag{3.11}$$

By construction the set of functions

$$\left\{\phi^{\vec{q}}(t,s,l)\,\middle|\,q_1,q_2\in\left[0,\frac{2\pi}{N}\right];\ q_3\in[0,2\pi);\ t=1,2,\ldots,N;\ l=1,2,\ldots,L;\ s\in\mathscr{Z}\right\} \tag{3.12}$$

forms a basis of $S(\mathscr{R}_y)\times S(\mathscr{R}_z)$ and the elements of this symmetry-adapted basis are orthogonal in the following sense:

$$(\phi^{\vec{q}}(t,s,l),\phi^{\vec{q}\,'}(t',s',l'))=\text{const}\times\delta(\vec{q}-\vec{q}\,')\delta_{tt'}\delta_{ss'}\delta_{ll'}\ , \tag{3.13}$$

where the "normalization constant" can be determined easily. The sets

$$\{\phi^{\vec{q}}(t,s,l)\mid l=1,2,\ldots,L;\ s\in\mathscr{Z}\}$$

span the distinct invariant subspaces of $S(\mathscr{R}_y)\times S(\mathscr{R}_z)$, which will be denoted by $S_t^{\vec{q}}(\mathscr{R}_y,\mathscr{R}_z)$. The invariant subspaces of $S(\mathscr{R}^3)$ are then given by $S(\mathscr{R}_x)\times S_t^{\vec{q}}(\mathscr{R}_y,\mathscr{R}_z)$. The eigenvalue problem associated with $\mathscr{H}$ can be separately attacked within each of these function spaces. Moreover, because of the N-fold degeneracy of the eigenvalues, we may restrict the investigation to the subspaces $S(\mathscr{R}_x)\times S_1^{\vec{q}}(\mathscr{R}_y,\mathscr{R}_z)$: Once the first eigenfunction of the degeneracy space is found the others may be generated immediately using Eq. (3.6).

Defining the set of functions

$$\left\{\varphi(q_1,q_2,l;y)\,\middle|\,q_1,q_2\in\left[0,\frac{2\pi}{N}\right];\ l=1,2,\ldots,L\right\}$$

by

$$\phi^{\vec{q}}(1,s,l;y,z)\equiv\exp\left[i\frac{b_3^z}{\alpha^{1/2}}(q_3+2\pi s)z\right]\varphi(q_1,q_2,l;y)\ , \tag{3.14}$$

any element $\psi^{\vec{q}}(1;x,y,z)$ of $S(\mathscr{R}_x)\times S_1^{\vec{q}}(\mathscr{R}_y,\mathscr{R}_z)$ can be expanded in the following way:

$$\psi^{\vec{q}}(1;x,y,z)=\int_{-\infty}^{\infty}dx_0\sum_{s\in\mathscr{L}}\sum_{l=1}^{L}C(s,l;x_0)\delta(x-x_0)\exp\left[i\frac{b_3^z}{\alpha^{1/2}}(q_3+2\pi s)z\right]\varphi(q_1,q_2,l;y)$$

$$=\sum_{l=1}^{L}\left[\exp\left[i\frac{b_3^z}{\alpha^{1/2}}q_3z\right]\sum_{s\in\mathscr{L}}C(s,l;x)\exp\left[i\frac{b_3^z}{\alpha^{1/2}}2\pi sz\right]\right]\varphi(q_1,q_2,l;y)\ . \tag{3.15}$$

Let

$$F_l(x,z)\equiv\sum_{s\in\mathscr{L}}C(s,l;x)\exp\left[i\frac{b_3^z}{\alpha^{1/2}}2\pi sz\right]\ . \tag{3.16}$$

Then

$$\psi^{\vec{q}}(1;x,y,z)=\sum_{l=1}^{L}\left[\exp\left[i\frac{b_3^z}{\alpha^{1/2}}q_3z\right]F_l(x,z)\right]\varphi(q_1,q_2,l;y)\ , \tag{3.17a}$$

$$F_l(x,z+\alpha^{1/2}a_3^z)=F_l(x,z)\ . \tag{3.17b}$$

For a field-lattice geometry with $\vec{a}_1,\vec{a}_2\perp\vec{a}_3$ (3.17) represents the general separation ansatz leading to a reduction of the dimensionality of the problem. Special realizations of the separating functions $\varphi(q_1,q_2,l;y)$ have been used *ad hoc* in Refs. 1–5 to treat essentially two-dimensional model systems. Note that the $\varphi(q_1,q_2,l;y)$ by themselves constitute an orthogonal basis of $S(\mathscr{R}_y)$. They could have been generated directly from the basis $\{\,\delta(y-y_0)\,|\,y_0\in\mathscr{R}\,\}$ as symmetry-adapted functions with respect to the sub-ray-group of magnetic translations $\{\,T_M(n_1\vec{a}_1+n_2\vec{a}_2)\,|\,n_1,n_2\in\mathscr{L}\,\}$. For $\vec{a}_1\perp\vec{a}_2$ and $L=1$ the $\varphi(q_1,q_2,1)$ become the one-dimensional k-q functions[10] whose existence and properties are thus closely related to magnetic translation symmetry.

Inserting Eq. (3.17a) into the Schrödinger equation associated with (2.15) and using (2.16) and (2.17) we find:

$$\mathscr{H}\psi^{\vec{q}}(1;x,y,z)=\sum_{l'=1}^{L}\left[\left[\frac{\hbar\omega_c}{2}(p_x^2+x^2)+\frac{\hbar\omega_c}{2}p_z^2\right]\exp\left[i\frac{b_3^z}{\alpha^{1/2}}q_3z\right]F_{l'}(x,z)\right]\varphi(q_1,q_2,l';y)$$

$$+\sum_{l'=1}^{L}\sum_{\vec{G}}\left[v(\vec{G})X(\vec{G};x,p_x)Z(g_3;z)\exp\left[i\frac{b_3^z}{\alpha^{1/2}}q_3z\right]F_{l'}(x,z)\right][Y(\vec{G};y,p_y)\varphi(q_1,q_2,l';y)]$$

$$=E\psi^{\vec{q}}(1;x,y,z)=\exp\left[i\frac{b_3^z}{\alpha^{1/2}}q_3z\right]\sum_{l=1}^{L}[EF_l(x,z)]\varphi(q_1,q_2,l;y)\ . \tag{3.18}$$

The kinetic term, i.e., the first term on the right-hand side of Eq. (3.18), readily gives

$$\exp\left[i\frac{b_3^z}{\alpha^{1/2}}q_3z\right]\sum_{l=1}^{L}\left\{\sum_{l'=1}^{L}\left[\frac{\hbar\omega_c}{2}(p_x^2+x^2)+\frac{\hbar\omega_c}{2}\left[p_z+\frac{b_3^z}{\alpha^{1/2}}q_3\right]^2\right]\delta_{ll'}F_{l'}(x,z)\right\}\varphi(q_1,q_2,l;y)\ . \tag{3.19}$$

Regarding the potential term in the second line we observe that

$$Y(\vec{G};y,p_y)=\exp\left[i\pi\frac{N}{L}g_1g_2\right]\exp\left[-i\pi\frac{N}{L}\frac{a_1^y}{a_2^y}g_2^2\right]T_y\left[-\alpha^{1/2}\frac{N}{L}a_1^xg_2\right]$$

$$\times\exp\left[-i\alpha^{1/2}\frac{N}{L}a_1^yg_2y\right]\exp\left[i\alpha^{1/2}\frac{N}{L}a_2^yg_1y\right]\ , \tag{3.20}$$

for $\vec{a}_1,\vec{a}_2\perp\vec{a}_3$. Then, after a somewhat lengthy but straightforward calculation we find

$$Y(\vec{G};y,p_y)\varphi(q_1,q_2,l';y)=\sum_{l=1}^{L}A_{ll'}(q_1,q_2;g_1,g_2)\varphi(q_1,q_2,l;y)\ , \tag{3.21}$$

with

$$A_{ll'}(q_1,q_2;g_1,g_2)=\exp\left[i\pi\frac{N}{L}g_1g_2\right]\exp\left[i\frac{2\pi}{L}l'g_1\right]\exp\left[i\frac{N}{L}(q_2g_1-q_1g_2)\right]$$
$$\times\exp\left[i\left[q_1-\frac{a_1^y}{a_2^y}q_2\right]\left[\frac{l-l'}{L}\right]\right]\exp\left[i\frac{\pi}{NL}\frac{a_1^y}{a_2^y}(l'^2-l^2)\right]\delta_{l,l'+Ng_2}(\mathrm{mod}L)\ . \tag{3.22}$$

Thus the entire potential term becomes

$$\exp\left[i\frac{b_3^z}{\alpha^{1/2}}q_3z\right]\sum_{l=1}^{L}\left[\sum_{l'=1}^{L}\left[\sum_{\vec{G}}v(\vec{G})A_{ll'}(q_1,q_2;g_1,g_2)X(\vec{G};x,p_x)Z(g_3,z)\right]F_{l'}(x,z)\right]\varphi(q_1,q_2,l;y)\ . \tag{3.23}$$

Inserting Eqs. (3.19) and (3.23) into (3.18), dividing both sides by $\exp(ib_3^zq_3z/\alpha^{1/2})$, and comparing the "coefficients" of the orthogonal functions $\varphi(q_1,q_2,l)$ we arrive at the following set of coupled equations:

$$\sum_{l'=1}^{L}H_{ll'}^{\vec{q}}(x,p_x;z,p_z)F_{l'}(x,z)=EF_l(x,z),\quad l=1,2,\ldots,L\ , \tag{3.24}$$

where

$$H_{ll'}^{\vec{q}}(x,p_x;z,p_z)=\left[\frac{\hbar\omega_c}{2}(p_x^2+x^2)+\frac{\hbar\omega_c}{2}\left[p_z+\frac{b_3^z}{\alpha^{1/2}}q_3\right]^2\right]\delta_{ll'}$$
$$+\sum_{\vec{G}}v(\vec{G})A_{ll'}(q_1,q_2;g_1,g_2)X(\vec{G};x,p_x)Z(g_3;z)\ . \tag{3.25}$$

Defining the $L\times L$-matrix operator $\mathscr{H}^{\vec{q}}(x,p_x;z,p_z)$ by

$$(\mathscr{H}^{\vec{q}}(x,p_x;z,p_z))_{ll'}\equiv H_{ll'}^{\vec{q}}(x,p_x;z,p_z)\ , \tag{3.26}$$

Eq. (3.24) can be written

$$\mathscr{H}^{\vec{q}}(x,p_x;z,p_z)\vec{F}(x,z)=E\vec{F}(x,z)\ , \tag{3.27}$$

with $\vec{F}(x,z)=(F_1(x,z),\ldots,F_L(x,z))^T$, where the superscript T indicates the transpose.

This is the desired result: The original Hamiltonian (2.10) has been replaced without approximations by the set

$$\left\{\mathscr{H}^{\vec{q}}(x,p_x;z,p_z)\middle|q_1,q_2\in\left[0,\frac{2\pi}{N}\right],\ q_3\in[0,2\pi)\right\} \tag{3.28}$$

of two-dimensional equivalent matrix operators, which act on the space of vector functions $\vec{F}(x,z)$. Because of Eq. (3.17b) the coordinate z can be restricted to the domain [0,1). The y degree of freedom and all systematic degeneracy which is "transported" by the former, have vanished altogether from our eigenvalue problem.

Regarding the equivalent Schrödinger equations (3.27) we observe the following properties: Owing to the finite z domain and to the oscillator character of the kinetic part of the equivalent Hamiltonians with respect to the x coordinate the spectrum of each $\mathscr{H}^{\vec{q}}$ is discrete (see also Refs. 1–4). Therefore we classify the energy eigenvalues of a given $L\times L$-matrix operator $\mathscr{H}^{\vec{q}}$ by $E^{\vec{q}}(r,s,l)$ and the corresponding "eigenspinors" by $\vec{F}^{\vec{q}}(r,s,l;x,z)$. Here $r\in\mathscr{N}$, $s\in\mathscr{L}$, and $l=1,2,\ldots,L$ refer to the x, z, and "spin" degree of freedom, respectively. All eigenfunctions of $\mathscr{H}$ [as given by Eq. (2.15)] are then obtained by Eqs. (3.17a) and (3.6). They

will be denoted by $\psi^{\vec{q}}(t,r,s,l;x,y,z)$, where $t=1,2,\ldots,N$ counts the degenerate states. The classification parameters

$$q_1,q_2\in\left[0,\frac{2\pi}{N}\right),\quad q_3\in[0,2\pi)\ ,$$
$$r\in\mathcal{N},\quad s\in\mathcal{I}\ , \tag{3.29}$$
$$l=1,2,\ldots,L,\quad t=1,2,\ldots,N\ ,$$

which emerged quite automatically in the course of the reduction procedure together constitute a complete set of quantum numbers of the problem. As shown below this is also true for general (rational) field-lattice geometry.

Only with the conditions of this subsection that the magnetic field and hence the primitive vector $\vec{a}_3$ is perpendicular to two linearly independent lattice vectors is a further reduction of the eigenvalue problem to one dimension possible. Actually, additional requirements have to be made: If the variation of the crystal potential in Eq. (2.1) along the direction of $\vec{B}$ is neglected altogether (as has been done in Refs. 5 and 6) or if this variation is purely additive [i.e., $V(x,y,z)=W(x,y)+U(z)$, see Refs. 1–4], then Eq. (3.27) can be separated into independent one-dimensional equations. The decoupling of x and z degree of freedom is easily achieved by factorization of the spinor $\vec{F}(x,z)$ and leads to the results previously derived.[1–6]

B. Arbitrary field-lattice geometry

We now drop all restrictions of subsection A regarding crystal symmetry and orientation of the primitive vectors with respect to $\vec{B}$. We specify, however, our rational magnetic field by the condition

$$N=L=1\ . \tag{3.30}$$

The latter is done only for the sake of clarity; the generalization to arbitrary N and L along the lines of the previous subsection is quite clear.

Although we now have to deal with a much more complicated situation the decomposition of the preadapted basis (3.10) of $S(\mathcal{R}_y)\times S(\mathcal{R}_z)$ into irreducible function sets with the aid of the projection operators (3.8) is still straightforward. Because of Eq. (3.30) the different sets belonging to the same $D^{\vec{q}}$ are classified by only one index, i.e., $s\in\mathcal{I}$, and consist of a single function $\phi^{\vec{q}}(s;y,z)$ given by

$$\phi^{\vec{q}}(s;y,z)=\exp\left[i\frac{b_3^z}{\alpha^{1/2}}(q_3+2\pi s)z\right]\sum_m\exp\left[i\left[q_1-\frac{a_1^y}{a_2^y}q_2+a_1^x b_3^x(q_3+2\pi s)\right]m\right]$$
$$\times\exp\left[-i\frac{\alpha}{2}a_1^x a_1^y m^2\right]\delta\left[y-\alpha^{1/2}a_1^x m-\frac{\alpha^{1/2}}{2\pi}a_1^x q_2-\frac{b_3^y}{\alpha^{1/2}}(q_3+2\pi s)\right. \tag{3.31}$$

In deriving this extensive use of Eq. (2.8) has been made.

The sets $\{\phi^{\vec{q}}(s)\,|\,s\in\mathcal{I}\}$ span the invariant subspaces $S^{\vec{q}}(\mathcal{R}_y,\mathcal{R}_z)$ of $S(\mathcal{R}_y)\times S(\mathcal{R}_z)$. Thus the entire set of functions $\{\phi^{\vec{q}}(s)\,|\,q_1,q_2q_3\in[0,2\pi);\ s\in\mathcal{I}\}$ forms another symmetry-adapted basis of $S(\mathcal{R}_y)\times S(\mathcal{R}_z)$ [see Eqs. (3.12) and (3.13)] with the following orthogonality properties:

$$(\phi^{\vec{q}}(s),\phi^{\vec{q}\,'}(s'))=\text{const}\times\delta(\vec{q}-\vec{q}\,')\delta_{ss'}\ . \tag{3.32}$$

There is one important difference between the irreducible basis functions $\phi^{\vec{q}}(s;y,z)$ and their counterparts (3.11) of case A: As can be seen from Eq. (3.31) the y and the z coordinate are now coupled through the parameter s reflecting the physical interdependence of the two degrees of freedom for general field-lattice geometry. An arbitrary element $\psi^{\vec{q}}(x,y,z)$ of the invariant subspace $S(\mathcal{R}_x)\times S^{\vec{q}}(\mathcal{R}_y,\mathcal{R}_z)$ of $S(\mathcal{R}^3)$ has now the expansion

$$\psi^{\vec{q}}(x,y,z)=\sum_{s\in\mathcal{I}}C_s(x)\phi^{\vec{q}}(s;y,z)\ . \tag{3.33}$$

Inserting (3.33) into the Schrödinger equation associated with (2.15) and proceeding as in Sec. III A we are led, after some algebra, to the infinite set of coupled equations for the coefficient functions $C_s(x)$:

$$\sum_{s'}H_{ss'}^{\vec{q}}(x,p_x)C_{s'}(x)=EC_s(x),\quad s\in\mathcal{I} \tag{3.34}$$

where

$$H_{ss'}^{\vec{q}}(x,p_x)=\left[\frac{\hbar\omega_c}{2}(p_x^2+x^2)+\frac{\hbar\omega_c}{2}\frac{a_1^x a_2^y}{2\pi}(b_3^z)^2(q_3+2\pi s')^2\right]\delta_{ss'}$$

$$+\sum_{\vec{G}} v(\vec{G})A_{ss'}(\vec{q};\vec{G})X(\vec{G};x,p_x) \tag{3.35}$$

and

$$A_{ss'}(\vec{q};\vec{G})=\exp(-i\pi g_1 g_2)\exp(-iq_1 g_2+iq_2 g_1)\exp(ia_1^x b_3^x q_2 g_3)$$

$$\times\exp\{i[b_3^z(g_2 a_1^z-g_1 a_2^z)+a_1^x a_2^y b_3^x b_3^y g_3](q_3-\pi g_3+2\pi s)\}\delta_{s,s'+g_3}\,. \tag{3.36}$$

Equation (3.34) is equivalent to the spinor-Schrödinger equation

$$\mathscr{H}^{\vec{q}}(x,p_x)\vec{C}(x)=E\vec{C}(x)\,, \tag{3.37}$$

where the effective matrix operator $\mathscr{H}^{\vec{q}}$, which refers to the x degree of freedom only but has infinite "spin" dimension, is defined by

$$(\mathscr{H}^{\vec{q}}(x,p_x))_{ss'}\equiv H_{ss'}^{\vec{q}}(x,p_x)\,. \tag{3.38}$$

Of course $\vec{C}(x)=(C_1(x),C_2(x),\ldots)^T$.

In the next and final step we replace $\mathscr{H}^{\vec{q}}$ by an equivalent scalar operator which refers to two degrees of freedom instead. We introduce a new pseudocoordinate z', the corresponding momentum operator $p_z'=(1/i)(\partial/\partial z')$ and a unitary space of functions whose elements $F(x,z')$ have to satisfy the periodicity condition

$$F(x,z'+1)=F(x,z')\,. \tag{3.39}$$

Then, let

$$\overline{\mathscr{H}}^{\vec{q}}(x,p_x;z',p_z')\equiv\frac{\hbar\omega_c}{2}(p_x^2+x^2)+\frac{\hbar\omega_c}{2}\frac{a_1^x a_2^y}{2\pi}(b_3^z)^2(p_z'+q_3)^2$$

$$+\sum_{\vec{G}} v(\vec{G})\exp(-i\pi g_1 g_2)\exp[-iq_1 g_2+iq_2(g_1+a_1^x b_3^x g_3)]$$

$$\times\exp\{i[b_3^z(g_2 a_1^z-g_1 a_2^z)+a_1^x a_2^y b_3^x b_3^y g_3](q_3+\pi g_3)\}$$

$$\times X(\vec{G};x,p_x)\exp(i2\pi g_3 z')T_{z'}(b_3^z(g_2 a_1^z-g_1 a_2^z)+a_1^x a_2^y b_3^x b_3^y g_3) \tag{3.40}$$

be an operator, which acts on that space.

The Schrödinger equation associated with $\overline{\mathscr{H}}^{\vec{q}}(x,p_x;z',p_z')$ is equivalent to Eq. (3.37). This can be checked immediately expanding $F(x,z')$ as

$$F(x,z')=\sum_{s'\in\mathscr{Z}} C_{s'}(x)\exp(i2\pi s'z') \tag{3.41}$$

and verifying

$$\int_0^1 dz'[\exp(i2\pi sz')]^*\overline{\mathscr{H}}^{\vec{q}}(x,p_x;z',p_z')\exp(i2\pi s'z')=H_{ss'}^{\vec{q}}(x,p_x)\,. \tag{3.42}$$

Thus, also in the most general (rational) case we have succeeded in eliminating the y degree of freedom: The set of two-dimensional Hamiltonians $\overline{\mathscr{H}}^{\vec{q}}(x,p_x;z',p_z')$, classified by the wave vector $\vec{q}$ of the magnetic Brillouin zone, describes the dynamics of our system completely. Obviously all comments given in the preceding section concerning the quantum numbers of the problem remain valid.

IV. PROPERTIES OF THE DIAMAGNETIC WAVE FUNCTIONS

One of the most intricate points within this whole field of research is the structure of the diamagnetic wave functions. Many questions arise: What is the global behavior of the stationary solutions under the competitive influence of the localizing magnetic field and the dispersing crystal potential; how is the local shape of the wave functions determined by electrostatic and magnetic forces respectively; how are the limiting cases of Bloch functions and free magnetic solutions realized when either the magnetic field or the periodic potential vanishes, etc.?

We have gained in Sec. III a great deal of explicit information on the "equivalent" diamagnetic solutions. This information, together with certain results of model calculations,[2,4] can be used to reveal the structure of the "true" physical wave functions. To this end we will first derive formulas describing how functions of the coordinates transform there and back when phase space is rotated according to Eq. (2.13).

As the canonical transformation (2.13) does not mix the first two degrees of freedom with the third one and as the partial transformation with respect to the latter is trivial we have to deal, in this regard, only with a two-dimensional problem. Then both $\{x,y\}$ and $\{\tilde{x},\tilde{y}\}$ constitute a complete set of commutating observables and the corresponding simultaneous "orthonormal" eigenstates can be characterized unambiguously by the kets $|\xi,\eta\rangle$ and $|\tilde{\xi},\tilde{\eta}\rangle$, respectively. Thus we have

$$\begin{aligned} &x\,|\xi,\eta\rangle=\xi\,|\xi,\eta\rangle,\quad y\,|\xi,\eta\rangle=\eta\,|\xi,\eta\rangle\ , \\ &\qquad\qquad \xi,\eta\in\mathscr{R}\ , \\ &\tilde{x}\,|\tilde{\xi},\tilde{\eta}\rangle=\tilde{\xi}\,|\tilde{\xi},\tilde{\eta}\rangle,\quad \tilde{y}\,|\tilde{\xi},\tilde{\eta}\rangle=\tilde{\eta}\,|\tilde{\xi},\tilde{\eta}\rangle\ , \\ &\qquad\qquad \tilde{\xi},\tilde{\eta}\in\mathscr{R}\ , \end{aligned} \tag{4.1a}$$

$$\begin{aligned} &\langle\xi,\eta\,|\,\xi',\eta'\rangle=\delta(\xi-\xi')\delta(\eta-\eta') \\ &\langle\tilde{\xi},\tilde{\eta}\,|\,\tilde{\xi}',\tilde{\eta}'\rangle=\delta(\tilde{\xi}-\tilde{\xi}')\delta(\tilde{\eta}-\tilde{\eta}')\ . \end{aligned} \tag{4.1b}$$

Obviously the old and the new coordinate representations of a general Hilbert space vector $|\phi\rangle$ are connected in the following way:

$$\phi(\xi,\eta)=\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}d\tilde{\xi}\,d\tilde{\eta}\,\langle\xi,\eta\,|\,\tilde{\xi},\tilde{\eta}\rangle\tilde{\phi}(\tilde{\xi},\tilde{\eta})\ , \tag{4.2}$$

where

$$\phi(\xi,\eta)\equiv\langle\xi,\eta\,|\,\phi\rangle,\quad \tilde{\phi}(\tilde{\xi},\tilde{\eta})\equiv\langle\tilde{\xi},\tilde{\eta}\,|\,\phi\rangle\ .$$

The kernel $f_{\tilde{\xi},\tilde{\eta}}(\xi,\eta)\equiv\langle\xi,\eta\,|\,\tilde{\xi},\tilde{\eta}\rangle$ of this unitary integral transformation is easily determined: Eqs. (4.1a) and (2.13a) together yield

$$\tilde{\xi}\,|\,\tilde{\xi},\tilde{\eta}\rangle=\tilde{x}\,|\,\tilde{\xi},\tilde{\eta}\rangle=\left[\frac{\alpha^{1/2}}{2}x-\frac{\alpha^{-1/2}}{\hbar}p_y\right]|\,\tilde{\xi},\tilde{\eta}\rangle\ . \tag{4.3}$$

"Multiplying" this equation by $\langle\xi,\eta\,|$ we get

$$i\alpha^{-1/2}\frac{\partial f_{\tilde{\xi},\tilde{\eta}}(\xi,\eta)}{\partial\eta}=\left[\tilde{\xi}-\frac{\alpha^{1/2}}{2}\xi\right]f_{\tilde{\xi},\tilde{\eta}}(\xi,\eta)\ . \tag{4.4a}$$

On the other hand, setting up for $\tilde{y}$ a relation similar to Eq. (4.3), one obtains

$$i\alpha^{-1/2}\frac{\partial f_{\tilde{\xi},\tilde{\eta}}(\xi,\eta)}{\partial\eta}=\left[\frac{\alpha^{1/2}}{2}\xi-\tilde{\eta}\right]f_{\tilde{\xi},\tilde{\eta}}(\xi,\eta)\ . \tag{4.4b}$$

Subtracting and adding Eqs. (4.4a) and (4.4b) we arrive at the system of equations

$$\begin{aligned} &(\tilde{\xi}+\tilde{\eta}-\alpha^{1/2}\xi)f_{\tilde{\xi},\tilde{\eta}}(\xi,\eta)=0\ , \\ &\frac{\partial f_{\tilde{\xi},\tilde{\eta}}(\xi,\eta)}{\partial\eta}=\frac{i\alpha^{1/2}}{2}(\tilde{\eta}-\tilde{\xi})f_{\tilde{\xi},\tilde{\eta}}(\xi,\eta)\ , \end{aligned} \tag{4.5}$$

which is solved by

$$\begin{aligned} f_{\tilde{\xi},\tilde{\eta}}(\xi,\eta)=C\exp&\left[i\frac{\alpha^{1/2}}{2}(\tilde{\eta}-\tilde{\xi})\eta\right] \\ &\times\delta(\xi-\alpha^{-1/2}(\tilde{\xi}+\tilde{\eta}))\ , \end{aligned} \tag{4.6}$$

C being a constant of integration. The latter is determined by condition (4.1b) up to a phase factor and will be chosen as $(1/2\pi)^{1/2}$.

Reintroducing the symbols x,y,z and $\tilde{x},\tilde{y},\tilde{z}$ for the old and the new coordinates, respectively, and using Eqs. (4.2), (4.6), and (2.13) we find that the original and the equivalent three-dimensional wave functions transform into each other in the following way:

$$\psi(x,y,z)=\frac{\alpha^{1/4}}{(2\pi)^{1/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}d\tilde{x}\,d\tilde{y}\exp\left[i\frac{\alpha^{1/2}}{2}(\tilde{y}-\tilde{x})y\right]\delta(x-\alpha^{-1/2}(\tilde{x}+\tilde{y}))\tilde{\psi}(\tilde{x},\tilde{y},\alpha^{1/2}z) \tag{4.7a}$$

$$\tilde{\psi}(\tilde{x},\tilde{y},\tilde{z})=\frac{\alpha^{-1/4}}{(2\pi)^{1/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dx\,dy\exp\left[-i\frac{\alpha^{1/2}}{2}(\tilde{y}-\tilde{x})y\right]\delta(x-\alpha^{-1/2}(\tilde{x}+\tilde{y}))\psi(x,y,\alpha^{-1/2}\tilde{z})\ . \tag{4.7b}$$

Obviously, this is the hybrid of a coordinate-coordinate and a coordinate-momentum transformation.

We are now able to describe the global and local structure of the "true" stationary states of our problem. This will be demonstrated for the familiar model system[11-14,1,2,4] consisting of a square lattice with lattice constant a in the x-y plane and a rational magnetic field $\vec{B}=B\hat{z}$ characterized by $L=1$ (arbitrary N). For this system Eq. (2.8c) simply becomes

$$\alpha=\frac{2\pi}{a^2}\frac{1}{N} \tag{4.8}$$

and, according to Eqs. (3.17a), (3.11), (3.14), (4.8), and (3.29), all the first-partner wave functions in rotated phase space read

$$\tilde{\psi}^{(q_1,q_2)}(1,r;\tilde{x},\tilde{y})=F^{(q_1,q_2)}(r;\tilde{x})\varphi(q_1,q_2;\tilde{y}),\quad q_1,q_2\in[0,\alpha a^2),\quad r\in\mathcal{N} \tag{4.9}$$

with

$$\varphi(q_1,q_2;\tilde{y})=\sum_{m\in\mathcal{Z}}\exp(iq_1m)\delta\left[\tilde{y}-\alpha^{1/2}a(m+1)-\frac{q_2}{\alpha^{1/2}a}\right]. \tag{4.10}$$

The $F^{(q_1,q_2)}(r;\tilde{x})$ in Eq. (4.9) are square-integrable solutions of the reduced equivalent Schrödinger equations corresponding to (3.27) under the prevailing conditions. From (3.13) we have on the other hand: $||\varphi(q_1,q_2;\tilde{y})||^2\propto\delta(0)^2$. Applying the transformation formula (4.7a) to $\tilde{\psi}^{(q_1,q_2)}(1,r)$ and defining

$$k_y(m,q_2)\equiv\alpha am+q_2/a\ , \tag{4.11}$$

we find

$$\psi^{(q_1,q_2)}(1,r;x,y)=\left[\frac{\alpha}{2\pi}\right]^{1/2}\exp(-iq_1)\exp\left[-i\frac{\alpha}{2}xy\right]\sum_{m\in\mathcal{Z}}\exp(iq_1m)\exp[ik_y(m,q_2)y]$$
$$\times F^{(q_1,q_2)}(r;\alpha^{1/2}[x-k_y(m,q_2)/\alpha])\ . \tag{4.12}$$

We do not calculate here the other $N-1$ partner functions as the first one is full representative for our considerations.

First we observe from Eq. (4.12) that the "true" rational-field wave functions are definitely Bloch-type states, extended with respect to all coordinates. This is a reasonable result, because the degeneracy spaces are of finite dimension and group theory predicts that all solutions can be chosen as extended ones. Note the strange property of the canonical transformation (2.13) and (4.7) to redistribute the amplitude of the original wave function in an extreme asymmetric way among the new coordinates and vice versa.

Let us now look at the structural details of the wave functions: The actual diamagnetic solutions essentially are composed of shifted replica of a localized function $F^{(q_1,q_2)}(r;\alpha^{1/2}x)$, centered around all lattice sites along the x axis [see Eq. (4.11)] and multiplied by plane wave factors referring to the y degree of freedom. The global behavior is a direct consequence of the field-lattice geometry; the dependence on the individual shape of the crystal potential is exclusively felt through the "generating" function $F^{(q_1,q_2)}(r)$, which contains all information regarding the energy eigenvalues.

Now, as indicated by extensive[2,4] model calculations, $F^{(q_1,q_2)}(r;\alpha^{1/2}x)$ by itself is (at least as far as the center of the magnetic Brillouin zone is concerned) the superposition of strongly localized functions of separation Na. The latter are shifted oscillator functions of a fixed level, periodically modulated in a way which is prescribed by the periodic potential actually chosen.

Thus the diamagnetic wave functions $\psi^{(q_1,q_2)}(1,r;x,y)$ exhibit at least two characteristic quasiperiods with respect to the x coordinate, namely the lattice constant a and a superlattice constant Na, and may be generated, in principle, from one single oscillator function by appropriate

translation and modulation.

When the crystal potential is "switched off" $F^{(q_1,q_2)}(r)$ reduces to the rth pure oscillator function [see (3.27)]; so $\psi^{(q_1,q_2)}(1,r)$ obviously becomes a linear combination of shifted degenerated free Landau functions, which is symmetry-adapted to the empty lattice.

As is well known the limit of vanishing magnetic field cannot be performed in such a continuous way: Actually, this limit here means $N \to \infty$ and, as a consequence, infinite degeneracy of each energy level at each point of the magnetic Brillouin zone, which at the same time shrinks to zero area.

The above qualitative analysis for the diamagnetic wave functions applies, in its main features, also to the general case of arbitrary crystal potential and rational field. Quantitative analytical and numerical results for selected situations are planned to be presented in a forthcoming paper.

V. CONCLUDING REMARKS

By means of the methods developed in this paper the quantum-mechanical treatment of Bloch electrons in magnetic fields can be greatly simplified for all crystals and all rational fields. In particular, it is shown how a reduction of the dimensionality of the problem is achieved in a direct and transparent way even in the case of genuine three-dimensional systems which usually must be dealt with. As a remarkable fact it turns out that properly generalized k-q functions[10,3] constitute a natural and powerful device to take full account of magnetic translation symmetry.

These results pave the way to an extension of first-principles calculations[1-4] to more complicated situations than hitherto considered. For instance, the dependence of the diamagnetic subband structure on the motion along the field can be studied by inspection of (simple) model systems, e.g., two-dimensional lattices with a rational magnetic field slightly tilted with respect to the lattice plane normal. As an even more rewarding task the rigorous treatment of realistic systems seems to be feasible now. This would be of interest, in the first place, regarding semiconducting materials, where experimental data are abundant, yet the theory to explain them is still largely restricted to the semiclassical approach of the Peierls-Onsager dynamics.[15-17]

As to the computational techniques involved, such first-principles calculations can be performed by applying to the equivalent Schrödinger equations of reduced dimensionality either the variational method introduced in Refs. 1, 2, and 4 or second-order perturbation theory, which has been shown to give excellent results in the Landau region.[18]

Regarding the diamagnetic wave functions, their properties have become sufficiently clear now in the general rational case. Explicit model calculations for representative systems can complete the investigations made above. It should, however, always be kept in mind that "nearly all" fields (in the sense of number theory) are irrational ones, implying $N \to \infty$ and infinite degeneracy. Thus there is "always" considerable freedom in forming special linear combinations of the ubiquitous extended solutions. But even then it is not at all evident that stationary states localized within the plane perpendicular to the magnetic field can be constructed as is possible for electron motion in an arbitrary field and zero periodic potential[19]: The degeneracy is not of the same measure in these two situations. This is related to the fact that the Hamiltonian commutes with the crystalline magnetic translation group in one case but with the continuous magnetic translation group, which is much larger, in the other case.

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