First-principles calculation of diamagnetic band structure. I. Reduction to a one-dimensional Schrödinger equation

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We present a new first-principles attack on the problem of Bloch electrons in a magnetic field which, being rigorous, preserves all symmetries and in particular all predictions of the magnetic translation group. In this first paper we show that the problem can be reduced for a wide class of crystal symmetries and for magnetic fields that are rational in the sense of group theory to a one-dimensional Hamiltonian. This is done in two steps: First we introduce a canonical transformation that diagonalizes the free-electron part of the "magnetic Hamiltonian." An analysis of the transformed crystal potential for simple rational fields allows a separation ansatz in terms of k-q functions in one of the variables. The result is a set of Schrödinger equations in the remaining variables which have the structure of differential difference equations with periodic coefficients; they are solved in the accompanying paper.

I. INTRODUCTION

This and the following paper, quoted as papers I and II, give an extensive account of our exact quantum-mechanical calculation of the spectrum and wave functions of crystalline electrons in a homogeneous magnetic field.

The 1930's and 40's saw the quantum-mechanical explanation of diamagnetism and of the magneto-oscillatory effects on the basis of the free-electron Fermi gas. The results were only in qualitative agreement with experiments on most real metals; obviously band effects had to be accounted for; something like the effective-mass approximation which had been so successful in the electric-field case had to be found. This was achieved by Onsager[1] with the famous Peierls-(Luttinger)-Onsager hypothesis which assumes a (near) stability of the Bloch bands under the action of a magnetic field; the proposed procedure is as follows: In the dispersion $\epsilon_n(\vec{p}/\hbar)$ of the nth unperturbed Bloch band the crystal momentum $\hbar\vec{k}=\vec{p}$ is replaced by the kinetic momentum $\vec{p}-(e/c)\vec{A}$ and the resulting effective Hamiltonian

$$H_{\text{eff}}=\epsilon_n\left[\frac{1}{\hbar}\left(\vec{p}-\frac{e}{c}\vec{A}(\vec{r})\right)\right] \tag{1}$$

is treated semiclassically, i.e., as the classical Hamilton function of a pseudosystem that yields the classical equations of motion

$$\dot{\vec{r}}=\vec{v}_n(\vec{k})=\frac{1}{\hbar}\vec{\nabla}_{\vec{k}}\epsilon_n(\vec{k}),$$

$$\hbar\dot{\vec{k}}=\frac{e}{c}\vec{v}_n(\vec{k})\times\vec{B}.$$

Requantization via Bohr-Sommerfeld produces a discrete spectrum of magnetic orbits within each given Bloch band, often called Landau orbits.

The assumption (1) of H_{eff} appears at first rather *ad hoc*; yet it was justified by its fabulous practical success: Most of our extensive knowledge on the topology and size of Fermi surfaces in metals and semiconductors is based on the application of (1) (and confirmed by a few independent methods); some practical problems with degenerate bands and with "magnetic breakthrough" have been explained by additional reasonable assumptions; cf. Refs. 2 and 3, respectively.

In spite of this convincing explanatory power all the considerable efforts toward a quantum-mechanical first-principles derivation of the Peierls-Onsager method (for a review see, e.g., Refs. 4 and 5) were only partially successful for reasons that have begun to be understood lately. In fact the analytic, numerical, and group-theoretical evidence will be presented in paper II and in a planned forthcoming paper that, in spite of the excellent agreement of many experiments with the energies calculated from (1), the eigenspace of the operator H_{eff} is not at all equivalent with a well defined subset of the eigenfunctions of the exact single-particle Hamiltonian

$$H=(\vec{p}-e\vec{A}/c)^2/2m+V_{\text{per}}(\vec{r}). \tag{2}$$

Indeed (2) represents one of the few unsolved problems of one-particle quantum mechanics for two characteristic reasons: (a) The kinetic-energy part H_0 enforces square-integrable—in fact Gaussian—behavior of the wave function in at least one direction, whereas the periodic potential V_{per} would require Bloch waves in all directions. (b) The Landau orbits belonging to H_0 prescribe one characteristic length, e.g., the free-electron ground-state cyclotron radius, and the lattice prescribes another one; in general these lengths are incommensurate. All difficulties with (2) can be traced back to one of these properties.

Here we introduce a new, direct attack on (2), part of which was sketched in a recent letter[6] (see also Ref. 7): Based on the high-field approach developed recently,[8-10] we have been able to reduce the essential part of the problem posed by (2) to a one-variable eigenvalue problem; this will be worked out in paper I. Exact solutions of the resulting differential difference equation for the simplest nontrivial model crystal will be presented in paper II and compared extensively with the semiclassical Peierls-Onsager spectrum for the same case; agreements and disagreements serve to illustrate the usefulness and limits of the semiclassical method. What appears more important is that the new method opens the way to exact *ab initio* magnetic band-structure calculations for arbitrary fields and crystal potentials.

II. A CANONICAL TRANSFORMATION

The Hamiltonian we wish to treat is that of a single electron in a periodic potential and in the vector potential belonging to a homogeneous field $\vec{B}=B\hat{z}$:

$$H=\frac{1}{2m}\left(\vec{p}-\frac{e}{c}\vec{A}\right)^2+V_{\rm per}(x,y,z)\,. \tag{3}$$

$\vec{A}$ will be chosen in the symmetric gauge

$$\vec{A}=\tfrac{1}{2}B(-y,x,0)\,. \tag{4}$$

The free-electron or kinetic-energy part of (3) is then

$$H_0=\frac{1}{2m}\left[\left(p_x+\frac{eB}{2c}y\right)^2+\left(p_y-\frac{eB}{2c}x\right)^2+p_z^2\right]. \tag{5}$$

This Hamiltonian couples, in a well-known way, the x and the y degrees of freedom.

With the usual definitions

$$\omega_c=\frac{eB}{mc}\,,\quad \alpha=eB/\hbar c\,, \tag{6}$$

we rewrite H_0 as follows:

$$H_0=\frac{\hbar\omega_c}{2}\left[\left(\alpha^{-1/2}\frac{p_x}{\hbar}+\alpha^{1/2}\frac{y}{2}\right)^2+\left(\alpha^{-1/2}\frac{p_y}{\hbar}-\alpha^{1/2}\frac{x}{2}\right)^2\right]+\frac{p_z^2}{2m}\,. \tag{7}$$

As a first step toward the desired separation of H we will, in this paragraph, reduce this kinetic-energy part H_0 to the sum of two one-dimensional operators: the z motion and a degenerate harmonic oscillator. This is achieved by means of the following canonical transformation:

$$P=\alpha^{-1/2}\frac{p_x}{\hbar}+\alpha^{1/2}\frac{y}{2}\,,\quad p=\alpha^{-1/2}\frac{p_x}{\hbar}-\alpha^{1/2}\frac{y}{2}\,,$$
$$Q=-\alpha^{-1/2}\frac{p_y}{\hbar}+\alpha^{1/2}\frac{x}{2}\,,\quad q=\alpha^{-1/2}\frac{p_y}{\hbar}+\alpha^{1/2}\frac{x}{2}\,. \tag{8a}$$

Hence

$$x=\alpha^{-1/2}(Q+q)\,,\quad y=\alpha^{-1/2}(P-p)\,. \tag{8b}$$

Equation (8) preserves the canonical commutation rules

$$[Q,P]=i\,,\quad [q,p]=i\,,$$
$$[Q,p]=[q,P]=[Q,q]=[P,p]=0\,.$$

Inserting (8a) in (7) yields the desired result: The (p,q) degree of freedom is no longer explicitly exhibited in H_0, where

$$H_0=\tfrac{1}{2}\hbar\omega_c(P^2+Q^2)+p_z^2/2m\,. \tag{9}$$

Equation (9) produces, as it must, the free-electron Landau spectrum: Apart from the z motion it represents a one-dimensional harmonic oscillator which is infinitely degenerate with respect to a second degree of freedom—in this case the (p,q) motion.

Turning again to the full Hamiltonian we insert (8b) in the potential and obtain, in the new canonical variables,

$$V_{\rm per}=V_{\rm per}(\alpha^{-1/2}(Q+q),\,\alpha^{-1/2}(P-p),z)\,. \tag{10}$$

Thus, so far, we have apparently only shifted the problem of the coupled degrees of freedom from H_0 in the old x-y representation to $V_{\rm per}$ in the new q-Q representation. As we shall see, however, this representation offers, under the "rational" circumstances to be described presently, the ansatz for a complete separation of variables.

III. SEPARATION OF VARIABLES

At this point it proves necessary to specify the geometry with respect to the lattice: One has to invoke the concept of rational magnetic fields, first introduced by Brown.[11] A rational field lies along some integer lattice vector $\vec{R}$ and fulfills the condition

$$\vec{\alpha}=\frac{e}{\hbar c}\vec{B}=\frac{2\pi}{\Omega}\frac{L}{N}\vec{R}\,, \tag{11}$$

where N, L are integers without a common divisor and Ω is the volume of the unit cell. Almost all fields, of course, are irrational, but the rational fields form a denumerable infinite set which is dense everywhere. Moreover, the continuity arguments first proposed by Brown[12] have been substantiated in[13] at least in the high-field limit (i.e., only one free Landau level split up and broadened by the periodic potential): The spectrum, consisting of L subbands, depends indeed most drastically on the rational number L/N; the integrated density of states and similar macroscopically observable quantities, however, are nearly identical for close-by values of L/N

like $\frac{1}{3}$ and $\frac{11}{34}$.

If in the following only rational fields will be investigated, this should therefore—at least for all practical purposes—not mean any serious restriction. (The intriguing problem of finite versus infinite degeneracy for rational and irrational fields, respectively, has been considered, among others, by Rauh, Wannier, and Obermair[8] and shall only be taken up in paper II.) If one is willing to accept,

If one is willing to accept moreover, that the variation of the periodic potential along the field or z direction affects only the coarse or large scale structure of the spectrum—large gaps and some nonlinear rearrangement of the magnetic fine structure—and may therefore be neglected altogether for the study of this fine structure, then, as found independently by Wannier,[14] the separation in the remaining two variables can be achieved for all crystal structures, provided only $\vec{B}$ obeys (11). In fact it may very well be that the z dependence of the potential is of little relevance for the fine structure; for a rigorous treatment, however, we shall here further restrict the geometry of the field and the lattice: We want the z dependence of the potential to be additive and thus exactly separable at least in the lowest approximation.

For this purpose a lattice of at least monoclinic symmetry will be chosen, the magnetic field along its primative $\vec{a}_3$ vector and thus perpendicular to the $\vec{a}_1\vec{a}_2$ plane. Only in this case is it a plausible lowest approximation to set

$$V_{\text{per}}(x,y,z)=V_{1,2}(x,y)+V_3(z) \tag{12}$$

and hence, in the q-Q representation of paragraph 2,

$$H=\tfrac{1}{2}\hbar\omega_c(P^2+Q^2)+V_{1,2}(\alpha^{-1/2}(Q+q),\alpha^{-1/2}(P-p)) + \frac{1}{2m}p_z^2+V_3(z)=H_{1,2}+H_3\,. \tag{13}$$

H_3 produces a one-dimensional band structure $\epsilon_3(k_z)$ which has to be added to the magnetic spectrum $\epsilon_{1,2}$ now contained entirely in $H_{1,2}$. This two-dimensional Hamiltonian will now be treated exactly. For this purpose we expand the potential $V_{1,2}$ in a Fourier series:

$$V_{1,2}(x,y)=\sum_{h,k} v_{hk}\exp[i(h\vec{G}_1\cdot\vec{r}+k\vec{G}_2\cdot\vec{r})]\,. \tag{14}$$

Since $\vec{B}\parallel\vec{a}_3\parallel\hat{z}$, both $\vec{G}_1$ and $\vec{G}_2$ are in the xy plane and, without loss of generality, we may set

$$\vec{G}_1=G_1\hat{x}=\frac{2\pi\hat{x}}{a_1\sin\vartheta}\,, \qquad \vec{G}_2=-G_2\cos\vartheta\hat{x}+G_2\sin\vartheta\hat{y}=-\frac{2\pi\cos\vartheta}{a_2\sin\vartheta}\hat{x}+\frac{2\pi}{a_2}\hat{y}\,, \tag{15}$$

where

$$\vartheta=\sphericalangle(\vec{a}_1,\vec{a}_2)\,.$$

The two-variable Schrödinger equation that remains to be solved reads in the q-Q representation, where P and p are to be identified with $-i\partial/\partial Q$ and $-i\partial/\partial q$, respectively,

$$\left\{\tfrac{1}{2}\hbar\omega_c(P^2+Q^2)+\sum_{h,k}v_{hk}\exp\left[i\left(\frac{hG_1}{\alpha^{1/2}}(Q+q)+\frac{kG_2}{\alpha^{1/2}}[-(Q+q)\cos\vartheta+(P-p)\sin\vartheta]\right)\right]\right\}|\Psi(Q,q)\rangle=\epsilon_{1,2}|\Psi(Q,q)\rangle\,. \tag{16}$$

For the sake of clarity let us first take up the simplest case, that of an orthorhombic lattice, where $\vartheta=\pi/2$, $\cos\vartheta=0$, and the potential reads

$$V_{1,2}=\sum_{h,k}v_{hk}\exp\left[i\left(h\frac{G_1}{\alpha^{1/2}}(Q+q)+k\frac{G_2}{\alpha^{1/2}}(P-p)\right)\right]. \tag{17}$$

So far we have only made use of the directional rationality of the field (i.e., along a shortest lattice vector $\vec{a}_3$) to split off the motion along the field. In order to produce an ansatz that separates also the remaining two degrees of freedom q and Q, we notice that the exponentials in (17) consist—with respect to the coordinate q—of translation operators $\exp(-ikG_2\alpha^{-1/2}p)$ and phase factors $\exp(ihG_1\alpha^{-1/2}q)$ which, owing to the rationality of the field contained in α, combine to a phase angle λ_{hk} that is a rational fraction of 2π: Consider the product λ_{hk} of the factor of p and of q in these expressions and observe (15):

$$\lambda_{hk}=\frac{hkG_1G_2}{\alpha}=\frac{4\pi^2hk}{a_1a_2\alpha}=hk\frac{4\pi^2a_3}{\Omega\alpha}\,.$$

Using the rationality condition (11), one obtains

$$i\lambda_{hk}=hk2\pi i\frac{N}{L}\,. \tag{18}$$

(Remember that N, L, and, of course, the Miller indices h,k are integers.) Equation (18) shows that the combined action of the translation operators and the phase factors in (17) closes onto itself after L steps as follows:

$$\exp(Li\lambda_{hk})=1\quad\forall\,h,k\,.$$

Following this observation, the separation ansatz is made in such a way that the q part of the wave function is Bloch type both under $\exp(iG_1\alpha^{-1/2}q)$ and $\exp(-iG_2\alpha^{-1/2}p)$. In doing so we have to distinguish two classes of rational fields which, following the terminology of Hofstadter,[15] we shall call (a) pure cases: $L=1$, and (b) general cases:

$L \neq 1$. The pure cases, of course, are no longer dense everywhere, but even for the largest technically available fields of several ten kG the pure cases still form a "relatively dense" set; in fact for a cubic lattice with $a = 2$ Å and $\vec{B}$ along a cubic axis, we have B in (G) $\approx 10^6 L/N$; thus the pure case $L/N = 1/10^4$ corresponds to $B \approx 100$ kG and the pure case $L/N = 1/(10^4 - 1)$ to $B \approx 100.01$ kG.

We construct the desired complete orthonormal set of Bloch-type functions; they are localized at one point within each lattice cell of a yet undetermined length ρ along the q axis (cf. Ref. 16):

$$|\kappa, \lambda\rangle_q = \left(\frac{\rho}{2\pi}\right)^{1/2} \sum_{m=-\infty}^{+\infty} e^{i\rho\kappa m} |\rho m + \lambda\rangle_q , \tag{19}$$

where

$$\kappa \in [0, 2\pi/\rho], \quad \lambda \in [0, \rho] \tag{19a}$$

and where $|\lambda\rangle_q$ is an appropriately normalized δ function with

$$q|\lambda\rangle_q = \lambda |\lambda\rangle_q . \tag{19b}$$

This normalization can in fact be chosen as $\langle\lambda'|\lambda\rangle_q = \delta(\lambda - \lambda')$ such that

$$\langle\kappa', \lambda'|\kappa, \lambda\rangle_q = \delta(\kappa - \kappa')\delta(\lambda - \lambda') . \tag{20}$$

One easily verifies the constituting properties of this set: We have

$$\exp(-i\rho p)|\rho m + \lambda\rangle_q = |\rho(m+1) + \lambda\rangle_q$$

and therefore

$$e^{-i\rho p}|\kappa, \lambda\rangle_q = e^{-i\rho\kappa}|\kappa, \lambda\rangle_q . \tag{21}$$

On the other hand, due to (19b),

$$e^{i\sigma q}|\kappa, \lambda\rangle_q = e^{i\sigma\lambda}|\kappa + \sigma, \lambda\rangle_q . \tag{22}$$

The Brillouin zone with respect to κ extends from 0 to $2\pi/\rho$; therefore, if $\rho\sigma = 2\pi N$, N integer, we have

$$|\kappa + \sigma, \lambda\rangle_q = |\kappa + (2\pi/\rho)N, \lambda\rangle_q \equiv |\kappa, \lambda\rangle_q . \tag{23}$$

Only in this case the $|\kappa, \lambda\rangle_q$ are simultaneous eigenfunctions of $\exp(-i\rho p)$ and $\exp(i\sigma q)$.

A. Separation for pure cases

Equation (23) is the starting point for the pure cases: Returning to the potential $V_{1,2}$ of (17) we now identify

$$\rho \equiv \alpha^{-1/2} G_2 , \quad \sigma \equiv \alpha^{-1/2} G_1 ,$$

$$\rho\sigma = G_1 G_2/\alpha = 2\pi N$$

by definition of a pure case (cf. Ref. 17); thus we have produced the conditions where Eq. (23) holds.

For the complete wave function $|\Psi(Q, q)\rangle$ we try

$$|\Psi\rangle = |\Phi\rangle_Q |\kappa, \lambda\rangle_q . \tag{24}$$

The Schrödinger equation becomes

$$\left(\tfrac{1}{2}\hbar\omega_c(P^2 + Q^2) + \sum_{h,k} v_{hk} \exp\{i[h\sigma(Q+q) + k\rho(P-p)]\} - \epsilon_{1,2}\right)|\Psi\rangle = 0 . \tag{25}$$

Now, due to Eqs. (21)–(24) and the fact that $[Q+q, P-p] = 0$, the terms of the potential applied to $|\Psi\rangle$ yield

$$\begin{aligned}\exp\{i[h\sigma(Q+q)]\}\exp\{i[k\rho(P-p)]\}|\Psi\rangle &= \exp\{i[h\sigma(Q+q)]\}\exp(-ik\rho\kappa)|\kappa, \lambda\rangle_q \exp[i(k\rho P)]|\Phi\rangle_Q \\ &= \exp\{i[h\sigma(Q+\lambda)]\}\exp\{i[k\rho(P-\kappa)]\}|\Phi\rangle_Q |\kappa, \lambda\rangle_q .\end{aligned} \tag{26}$$

Equation (26) shows that the q-dependent part of the wave function is reproduced unaltered by each term of the potential. But the kinetic-energy term does not act on $|\kappa, \lambda\rangle_q$ at all; since the $|\kappa, \lambda\rangle_q$ are linearly independent, we may therefore factorize (25) as

$$|\kappa, \lambda\rangle_q [H(P, Q) - \epsilon_{1,2}]|\Phi\rangle_Q = 0 .$$

The separation is achieved and, according to (25) and (26), the one-dimensional Hamiltonian that remains to be treated in paper II reads

$$\begin{aligned}H(P, Q) = {} & \tfrac{1}{2}\hbar\omega_c(P^2 + Q^2) \\ & + \sum_{h,k} v_{hk} \exp\{i[h\sigma(Q+\lambda)]\} \\ & \times \exp\{i[k\rho(P-\kappa)]\} .\end{aligned} \tag{27}$$

The variables p and q have dropped out altogether, leaving behind a parametric dependence of $H(P, Q)$ on the two wave numbers κ and λ that, by the construction (19) of the $|\kappa, \lambda\rangle_q$, span a magnetic Brillouin zone (MBZ) of area $(2\pi/\rho)\rho = 2\pi$. It is not hard to see, however, that $H(P, Q)$ and its eigenvalues $\epsilon_{1,2}(\kappa, \lambda)$ are periodic in λ not only with the period ρ, but also with the smaller period ρ/N, which subdivides the MBZ into N smaller "proper MBZ's" of area $2\pi/N$. Since the $|\kappa, \lambda\rangle_q$ from different such proper MBZ's are linearly independent, this result confirms the N-fold degeneracy of the spectrum as required by group theory.[11,17]

The result (27) holds for orthorhombic symmetry; for the more general monoclinic case

formulated in Eq. (16) we have to generalize the ansatz (19). Again we assume a "pure case" rational field along $\vec{a}_3$:

$$\vec{\alpha} = \frac{e\vec{B}}{\hbar c} = \frac{2\pi}{N\Omega}\vec{a}_3 \tag{28}$$

and we identify the coefficients that occur in the exponentials of (16) in the following way:

$$\rho \equiv \alpha^{-1/2} G_2 \sin\vartheta, \quad \sigma \equiv \alpha^{-1/2} G_1 ,$$

$\rho\sigma = 2\pi N$ because of (15) and (28); the (h,k) Fourier component of the potential then reads

$$V_{hk} = v_{hk} \exp\{i[(h\sigma - k\rho\cot\vartheta)(Q+q) + k\rho(P-p)]\}. \tag{29}$$

Now the generalization of (19) that takes care of the $\cot\vartheta$ term is as follows:

$$|\kappa,\lambda,\tau\rangle_q = \left(\frac{\rho}{2\pi}\right)^{1/2} \sum_m \exp[i(\rho\kappa m + \tau m^2)]\,|\rho m + \lambda\rangle_q \tag{30}$$

and

$$|\Psi(Q,q)\rangle = |\Phi\rangle_Q |\kappa,\lambda,\tau\rangle_q . \tag{31}$$

Acting on (31) with (29) then yields

$$V_{hk}|\Psi\rangle = \left(\frac{\rho}{2\pi}\right)^{1/2} v_{hk} \exp\{i[(h\sigma - k\rho\cot\vartheta)(Q+q)]\} \sum_m \exp[i(\rho\kappa m + \tau m^2)]\,|\rho(m+k)+\lambda\rangle e^{ik\rho P}|\Phi\rangle$$

$$= \left(\frac{\rho}{2\pi}\right)^{1/2} v_{hk} \sum_m \exp(i\{(h\sigma - k\rho\cot\vartheta)[\rho(m+k)+\lambda] + \rho\kappa m + \tau m^2\})$$
$$\times\, |\rho(m+k)+\lambda\rangle \exp[i(h\sigma - k\rho\cot\vartheta)Q]\, e^{ik\rho P}|\Phi\rangle$$

$$= \left(\frac{\rho}{2\pi}\right)^{1/2} v_{hk} \sum_m \exp[i(-k\rho^2 m\cot\vartheta + \rho\kappa m + \tau m^2 + \tau k^2 - 2\tau k m)]$$
$$\times\, |\rho m + \lambda\rangle \exp[i(h\sigma - k\rho\cot\vartheta)(Q+\lambda)]\, e^{ik\rho(P-\kappa)}|\Phi\rangle .$$

If we now set $\tau = -\frac{1}{2}\rho^2\cot\vartheta$, then the first and the last term in the first exponential cancel and $|\kappa,\lambda,\tau\rangle$ is reproduced up to phase factors

$$V_{hk}|\Psi\rangle = |\kappa,\lambda,\tau\rangle v_{hk} \exp(i\tau k^2) \exp[i(h\sigma - k\rho\cot\vartheta)(Q+\lambda)] \exp[ik\rho(P-\kappa)]\,|\Phi\rangle .$$

Again we have achieved the separation and obtained a one-dimensional Hamiltonian,

$$H(P,Q) = \tfrac{1}{2}\hbar\omega_c(P^2+Q^2) + \sum_{h,k} v_{hk} \exp[-(i/2)\rho^2 k^2\cot\vartheta] \exp[i(h\sigma - k\rho\cot\vartheta)(Q+\lambda)] \exp[ik\rho(P-\kappa)]. \tag{32}$$

The properties of $H(P,Q)$ mentioned following Eq. (27) hold also in this more general lattice symmetry.

B. Separation for general cases

To keep the length down these cases will only be treated for lattices of at least orthorhombic symmetry. Again we set $\rho = \alpha^{-1/2} G_2$, $\sigma = \alpha^{-1/2} G_1$; then $\rho\sigma = G_1 G_2/\alpha = 2\pi N/L$, where $L \neq 1$, by the definition of a general rational case and we try an ansatz using the $|\kappa,\lambda\rangle_q$.

According to (22) the terms $\exp(i\sigma q)$ in the crystal potential will now reproduce $|\kappa,\lambda\rangle_q$ only after L applications. We therefore define

$$\begin{aligned} &|\kappa,l,\lambda\rangle_q = |\kappa + l\sigma,\lambda\rangle_q = |\kappa + 2\pi Nl/L\rho,\lambda\rangle_q, \quad l = 0,1,\ldots,L-1 \\ &|\kappa,l+\mu L,\lambda\rangle_q \equiv |\kappa,l,\lambda\rangle_q \text{ for } \mu \text{ integer} \end{aligned} \tag{33}$$

and generalize the previous ansatz (24) to read

$$|\Psi\rangle = \sum_{l=0}^{L-1} |\kappa,l,\lambda\rangle_q |\Phi_l\rangle_Q , \tag{34}$$

where now $\kappa \in [0, 2\pi/\rho L)$. The Schrödinger equation is in complete analogy to the derivation in (26) and with $H_0 = \frac{1}{2}\hbar\omega_c(P^2+Q^2)$, dropping the subscripts q,Q,

$$(H-\epsilon_{1,2})|\Psi\rangle=0=\sum_{l=0}^{L-1}\left(|\kappa,l,\lambda\rangle(H_0-\epsilon_{1,2})|\Phi_l\rangle+\sum_{h,k}v_{hk}|\kappa,l+h,\lambda\rangle\exp[ih\sigma(Q+\lambda)]\exp[ik\rho(P-\kappa-l\sigma)]|\Phi_l\rangle\right). \tag{35}$$

Since the $|\kappa,l,\lambda\rangle$ are linearly independent, their coefficients must vanish individually; thus the terms V_{hk} of the potential with $h\neq 0$ mod$L$ connect $|\Phi_l\rangle$ with $|\Phi_{l-h}\rangle$ and we obtain L coupled equations for the state vectors $|\Phi_l\rangle$:

$$[\tfrac{1}{2}\hbar\omega_c(P^2+Q^2)-\epsilon_{1,2}]|\Phi_l\rangle+\sum_{h,k}v_{h,k}\exp[ih\sigma(Q+\lambda)]\exp\{ik\rho[P-\kappa-(l-h)\sigma]\}|\Phi_{l-h}\rangle=0. \tag{36}$$

In other words, we have an $L\times L$ matrix Hamiltonian $H_{ll'}$, the elements of which are of course operators acting on the L components $(|\Phi_0\rangle,\ldots,|\Phi_{L-1}\rangle)$. Notice that infinitely many Fourier components V_{hk} with $h=(l-l')+\mu L$, μ integer, contribute to the matrix element $H_{l,l'}$. Thus we obtain

$$H_{l,l'}=\tfrac{1}{2}\hbar\omega_c(P^2+Q^2)\delta_{ll'}+\sum_{\mu,k}v_{\mu L+l-l',k}\exp[i(l-l'+\mu L)\sigma(Q+\lambda)]\exp[ik\rho(P-\kappa-l'\sigma)],\quad l,l'=0,1,\ldots,L-1. \tag{37}$$

It can be shown in a straightforward manner that the spectrum associated with (37) is again N-fold degenerate irrespective of the value of L. For $L=1$ Eq. (37) reduces to the Hamiltonian (27) of the pure case, as it must. The high-field approximation, valid if the distance $\hbar\omega_c$ of the free Landau levels is large compared to their broadening and splitting by the potential, is easily obtained from (37) by taking matrix elements with respect to one, e.g., the lowest free Landau state. For the simplest nontrivial example, the square lattice with only 4 nonvanishing Fourier components of the potential $v_{\pm1,0}=v_{0,\pm1}=v$, one thus recovers the $L\times L$ ordinary matrix problem or, equivalently, the difference equation

$$\alpha_{m+1}+2\cos(\eta m+\lambda)\alpha_{m-1}=\tilde{\epsilon}\alpha_m,$$

with $\eta=\rho\sigma=2\pi N/L$, $\tilde{\epsilon}=e^{-\eta^2}\epsilon/v$, and Bloch wave number κ, which have been treated extensively in previous work from our group.[13,15,18] The exact treatment for low and high fields of the one-dimensional equivalent Hamiltonians derived here will be presented in the subsequent paper II.

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