SPLITTING OF A BLOCH BAND INTO MAGNETIC SUBBANDS?

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It is shown that there is no group-theoretical foundation for the statement that a Bloch band splits into an integer number of magnetic subbands when a magnetic field $\boldsymbol{H}$ is turned on.

The translational symmetry of the Bloch electron in a magnetic field $\boldsymbol{H}$ does not fit into the conventional group-theoretical framework for the following reason. If H_0 is the Hamiltonian of the Bloch electron with translational symmetry T_0 and H the corresponding Hamiltonian in the presence of the magnetic field $\boldsymbol{H}$ with translational symmetry T, then as is well known [1], T is not a subgroup of T_0. Because of this reason, conventional group-theoretical splitting of an energy level under symmetry lowering is not applicable to the problem of a Bloch electron in a magnetic field. As a consequence of this, it was agreed upon [1,2] that there is no good reason to believe that a Bloch band should split into N magnetic bands when a magnetic field is applied. Blount [3] challenges this statement and claims that "group theory does require that an isolated band be divided into N subbands in a magnetic field". In what follows we are going to prove that this is unfounded.

In conventional group theory there is a well defined framework for the splitting of energy levels under symmetry lowering [4]. Let us present here the main idea of this framework. A set of states ψ_1, ψ_2, ..., ψ_n corresponding to an energy level ϵ and forming a basis for an irreducible representation γ of the group G_0 forms also a basis for a representation (in general, reducible) of a subgroup G of G_0. For simplicity, let us assume that when restricted to G the representation γ contains two irreducible representations γ_1 and γ_2 of G with dimensions l_1 and l_2, corresponding ($l_1+l_2=n$). The bases ϕ_{1p} ($p=1, 2, ..., l_1$) and ϕ_{2q} ($q=1, 2, ..., l_2$) of these representations γ_1 and γ_2 are linear combinations of the states ψ_i, $i=1, 2, ..., n$:

$$\phi_{1p}=\sum_{i=1}^{n}\alpha_{pi}^{(1)}\psi_i,\quad \phi_{2q}=\sum_{i=1}^{n}\alpha_{qi}^{(2)}\psi_i\,. \tag{1}$$

In physical terms G_0 is the symmetry of the unperturbed Hamiltonian H_0, while G (subgroup of G_0) is the symmetry of the perturbed Hamiltonian H. The functions ϕ_{1p} and ϕ_{2q} are the symmetry adapted functions in the lowest order of perturbation theory for H. The perturbed Hamiltonian H *splits* the energy level ϵ into two levels ϵ_1 and ϵ_2 corresponding to the functions ϕ_{1p} and ϕ_{2q}, respectively. In applications of group theory to quantum mechanics this is what splitting of an energy level into two (or more) levels means. In particular, the functions ϕ_{1p} and ϕ_{2q} of the split-off levels are linear combinations (1) of the states ψ_i, $i=1, 2, ..., n$ of the unperturbed level. The claim of ref. [1] that a Bloch band is not required by symmetry to split into N magnetic subbands follows from the fact that the magnetic translation group is not a subgroup of the translation group and is therefore consistent with conventional group theory.

In ref. [3] it is explicitly stated that the symmetry in the presence of $\boldsymbol{H}$ is not a subsymmetry of the field-free problem, and that "the field-free symmetry group is intrinsically irrelevant to the problem with a field". The splitting argument of ref. [3] is therefore not based on conventional group theory as outlined in the previous paragraph where the group–subgroup relation is invoked. It is rather based on the concept of the regular representation of the magnetic translation group (MTG).

In what follows it is shown that the splitting argument of ref. [3] is unfounded.

Let $\tau(\boldsymbol{a})$ and $\tau(\boldsymbol{b})$ be the magnetic translations in a rectangular two-dimensional lattice with boundary conditions $\tau^{Ns_1}(\boldsymbol{a})=\tau^{Ns_2}(\boldsymbol{b})=1$. Here s_1 and s_2 are arbitrary integers and N appears in the rationality condition $e\boldsymbol{H}\cdot(\boldsymbol{a}\times\boldsymbol{b})/hc=l/N$ (for the sake of simplicity and without loss of generality we shall assume $l=1$). With these boundary conditions the MTG has $N^2s_1s_2$ magnetic translations. It is claimed in ref. [3] that these magnetic translations, when applied to an arbitrary function $\psi(x, y)$, induce an $N^2s_1s_2$-dimensional regular representation of the MTG. This claim does not seem to be correct. This is best seen on the example of a zero periodic potential, $V=0$. In the latter case one can choose ψ to be a product function $\psi_1(\pi_x)\psi_2(\pi_{cx})$ where

$$\boldsymbol{\pi}=\boldsymbol{p}+\frac{e}{2c}\boldsymbol{H}\times\boldsymbol{r}$$

is the kinetic momentum and

$$\boldsymbol{\pi}_c=\boldsymbol{p}-\frac{e}{2c}\boldsymbol{H}\times\boldsymbol{r}$$

is an infinitesimal magnetic translation. With the above boundary conditions the $\psi_2(\pi_{cx})$-space is Ns_1s_2-dimensional. What this means is that the magnetic translations, when applied to $\psi_1(\pi_x)\psi_2(\pi_{cx})$, will at best lead to an Ns_1s_2-dimensional representation (the magnetic translations act trivially on $\psi_1(\pi_x)$ because they commute with π_x) and not to an $N^2s_1s_2$-dimensional representation as claimed in ref. [3]. The statement of ref. [3] that the magnetic translations induce an $N^2s_1s_2$-dimensional regular representation of the MTG, when applied to an arbitrary function $\psi(x, y)$, is therefore not correct.

Our proof actually shows that Blount's claim "What function to use for $\psi(\boldsymbol{r}; 0)$ is not terribly important" is in contradiction with the choice of a well localized free electron function. Thus, our product function $\psi_1(\pi_x)\psi_2(\pi_{cx})$ in the xy-representation is the Dingle function for the lowest Landau level,

$$\psi(\boldsymbol{r})=\left(\frac{1}{2\pi\lambda^2}\right)^{1/2}\exp\left(-\frac{x^2+y^2}{4\lambda^2}\right). \qquad (2)$$

This function is well localized around $\boldsymbol{R}=0$ and it therefore satisfies Blount's localizability condition. However, as was shown above, the magnetic translations when applied to it will at best lead to Ns_1s_2 independent functions (despite the fact that the magnetic translation group contains $N^2s_1s_2$ independent translations!). This is therefore a counter-example to the above claim by Blount and it shows that it is terribly important which localized function one chooses.

As another example we consider the Wannier functions that Blount suggests as a set for constructing an induced representation of the magnetic translation group,

$$a(\boldsymbol{r}; \boldsymbol{R})\equiv\tau(\boldsymbol{R})a(\boldsymbol{r}; 0)\,, \qquad (3)$$

where $a(\boldsymbol{r}; 0)$ are the Wannier functions for the crystal in the absence of the magnetic field (the functions in (3) are used in the effective Hamiltonian theory). Let us show that $a(\boldsymbol{r}; \boldsymbol{R})$ are incompatible with the magnetic boundary conditions and can therefore not be used for constructing an induced representation when $\boldsymbol{H}\neq 0$. For a finite crystal $a(\boldsymbol{r}; 0)$ satisfies the Born–von Karman boundary conditions,

$$a(\boldsymbol{r}+Ns_1\boldsymbol{a}; 0)=a(\boldsymbol{r}+Ns_2\boldsymbol{b}; 0)=a(\boldsymbol{r}; 0)\,. \qquad (4)$$

Now, the Wannier functions $a(\boldsymbol{r}; \boldsymbol{R})$ in ref. [3] have to satisfy the magnetic boundary conditions. In particular, for $a(\boldsymbol{r}; 0)$, we have to have

$$\exp\left(\mathrm{i}\frac{eH}{2\hbar c}Ns_1ay\right)a(\boldsymbol{r}+Ns_1\boldsymbol{a}; 0)$$
$$=\exp\left(-\mathrm{i}\frac{eH}{2\hbar c}Ns_2bx\right)a(\boldsymbol{r}+Ns_2\boldsymbol{b}; 0)$$
$$=a(\boldsymbol{r}; 0)\,. \qquad (5)$$

From refs. [4] and [5] it follows that

$$\exp\left(\mathrm{i}\,\frac{eH}{2\hbar c}Ns_1ay\right)=\exp\left(-\mathrm{i}\,\frac{eH}{2\hbar c}Ns_2bx\right)=1\,. \qquad (6)$$

This means that the boundary conditions (4) and (5) become compatible only when x and y are quantized (they assume discrete values only), which is non-physical. We conclude that the Wannier functions $a(\boldsymbol{r};0)$ for $\boldsymbol{H}=0$ cannot satisfy the magnetic boundary conditions (5), and the set $a(\boldsymbol{r};\boldsymbol{R})$ in ref. [3] can therefore not be used for constructing an $N^2s_1s_2$-dimensional induced representation of the magnetic translation group. Blount's claim "It is also clear that when $\boldsymbol{B}=0$, we can take a Wannier function $a(\boldsymbol{r};0)$ for the free-field band suitably modified for pseudoperiodicity, generate $a(\boldsymbol{r},\boldsymbol{R})\equiv T(\boldsymbol{R})a(\boldsymbol{r};0)$ and thus obtain the regular representation of $\mathrm{T_M}$" is therefore incorrect as is proven by our second counter-example.

The conclusion is that group theory (neither conventional, nor regular representation arguments) does not lead to a splitting of a Bloch band into N magnetic subbands when a magnetic field $\boldsymbol{H}$ is turned on. Correspondingly, the agreed upon statement of refs. [1] and [2] stands as it is.

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