First-Principles Calculation of Diamagnetic Band Structure

In their recent Letter,[1] Schellnhuber and Obermair claim to have shown that the lowest band in a solid at zero magnetic field splits "into precisely N subbands" in the presence of a rational magnetic field. N is given by the relation

$$2\pi\hbar/m\omega_c = Na^2, \tag{1}$$

where m is the mass of the electron, ω_c is the cyclotron frequency, and a is the lattice constant. It is also claimed that this splitting "agrees fully with group theory and the effective-Hamiltonian concept."

To our knowledge neither group theory nor effective Hamiltonians lead to a splitting of an isolated band into precisely N magnetic subbands. Let us first discuss the effective-Hamiltonian approach. In this approach the splitting into N subbands was confirmed only approximately for a tight-binding model and for low magnetic fields[2] (large N). For a free electron (empty lattice) the width $\Delta\epsilon$ of the lowest two-dimensional band is $\Delta\epsilon = (\hbar^2/m)(\pi/a)^2$. The spacing between Landau levels is $\hbar\omega_c$. With the rationality relation (1) in mind we find that the free-electron band splits into $\frac{1}{2}\pi N$ magnetic subbands (and not N as is claimed in Ref. 1). For a general band of width $\Delta\epsilon$ the number of subbands should be $(\Delta\epsilon/\epsilon_g)N$, where $\epsilon_g = 2\pi\hbar^2/ma^2$, if the spacing between the subbands is the same. In Fig. 1 of Ref. 1 the spacing between the subbands seems to be the same. It should therefore follow that the lowest band in Ref. 1 should split into $(\Delta\epsilon/\epsilon_g)N$ magnetic subbands. Since the authors of Ref. 1 show that for $N = 8$ the splitting is precisely into 8 subbands, we conclude that the condition $\Delta\epsilon/\epsilon_g = 1$ is in some unclear way a part of their model.

The statement of Ref. 1 that group theory should lead to the splitting into N subbands does not seem to us to be correct. It is true that the magnetic Brillouin zone is N times smaller than the Brillouin zone of the same crystal for a zero magnetic field.[3] Correspondingly, the magnetic band has N times fewer states than a Bloch band. However, the magnetic operator symmetry is not a subgroup of the Bloch symmetry,[3] and one has therefore no grounds to claim that a Bloch band should split into N magnetic subbands when $B \neq 0$. Since the magnetic symmetry at $B \neq 0$ is not a subsymmetry of the problem for $B = 0$, Bloch states do not go over into magnetic Bloch states when B is turned on.

We would also like to comment on the "separation *Anzatz*" which is made in deriving the one-dimensional eigenvalue equation of Ref. 1. It is claimed that the wave function can be written as a product function (for $L = 1$)

$$\Phi(Q,q) = \Psi(Q)\psi(q). \tag{2}$$

We do not think that Eq. (2) actually separates the variables. The variables Q and q are always coupled when the periodic potential $V(x,y) \neq 0$. This is actually well known from previous work,[4] where it was shown that the space of functions $\Phi(Q,q)$ can be decomposed into spaces labeled by the eigenvalues $\kappa\lambda$ of the magnetic translations. With such a decomposition $\Psi(Q)$ in (2) depends explicitly on κ and λ. This is equivalent to saying that the variables in (2) cannot be separated because $\kappa\lambda$ carry the same information as q. The explicit form of Eq. (2) is

$$\Phi_{l\kappa\lambda}(Q,q) = \Psi_{l\kappa\lambda}(Q)\langle q|\,\kappa\lambda\rangle, \tag{3}$$

where the index l labels the eigenfunctions of the one-dimensional Hamiltonian, and $\langle q|\,\kappa\lambda\rangle$ is the distribution[5]

$$\langle q|\,\kappa\lambda\rangle = \left(\frac{\rho}{2\pi}\right)^{1/2} \sum_{m=-\infty}^{\infty} l^{i\rho\kappa m}\delta(q - \lambda - m\rho). \tag{4}$$

The explicit expression (3) shows that the variables Q and q are, in fact, not separated. The appearance of the distribution (4) couples Q and q via the eigenvalues $\kappa\lambda$. This is in agreement with the decoupling as discussed in Ref. 4.

Our concluding remark is that the main equation of Ref. 1 [Eq. (6) therein] has already been derived many years ago.[6]

I. Dana
J. Zak
Department of Physics
Technion–Israel Institute of Technology
Haifa 32000, Israel

Received 29 July 1981
PACS numbers: 71.25.Cx, 75.20.-g

[1]H. J. Schellnhuber and G. M. Obermair, Phys. Rev. Lett. 45, 276 (1980).
[2]D. R. Hofstadter, Phys. Rev. B 14, 2239 (1976).
[3]W. Opechowski and W. G. Tam, Physica (Utrecht) 42, 529 (1969).
[4]F. Bentosela, Nuovo Cimento B16, 115 (1973).
[5]G. M. Obermair and H. J. Schellnhuber, Phys. Rev. B 23, 5185 (1981).
[6]J. Zak, Phys. Rev. 136, A1647 (1964).