First-Principles Calculation of Diamagnetic Band Structure

In their recent Letter,\textsuperscript{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

\[ 2\pi \hbar / m \omega_c = Na^2, \]

where \( m \) is the mass of the electron, \( \omega_c \) 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\textsuperscript{2} (large \( N \)). For a free electron (empty lattice) the width \( \Delta \epsilon \) of the lowest two-dimensional band is \( \Delta \epsilon = (h^2/m)(\pi/a)^2 \). 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 \( \frac{1}{2} N \) magnetic subbands (and not \( N \) as is claimed in Ref. \textsuperscript{1}). For a general band with width \( \Delta \epsilon \) the number of subbands should be \( \langle \Delta \epsilon / \epsilon \rangle N \), where \( \epsilon_c = 2 \pi \hbar^2 / ma^2 \), if the spacing between the subbands is the same. In Fig. \textsuperscript{1} of Ref. \textsuperscript{1} the spacing between the subbands seems to be the same. It should therefore follow that the lowest band in Ref. \textsuperscript{1} should split into \( \Delta \epsilon / \epsilon \) \( N \) magnetic subbands. Since the authors of Ref. \textsuperscript{1} show that for \( N = 8 \) the splitting is precisely into \( 8 \) subbands, we conclude that the condition \( \Delta \epsilon / \epsilon \approx 1 \) is in some unclear way a part of their model.

The statement of Ref. \textsuperscript{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.\textsuperscript{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,\textsuperscript{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 sub-symmetry 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. \textsuperscript{1}. It is claimed that the wave function can be written as a product function (for \( L = 1 \))

\[ \Phi(Q,q) = \psi(Q) \psi(q). \]

We do not think that Eq. (2) actually separates the variables. The variables \( Q \) and \( q \) are always coupled when the periodic potential \( V(\kappa) \neq 0 \). This is actually well known from previous work,\textsuperscript{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 \( \kappa \) and \( \lambda \). 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

\[ \Phi(\kappa,\lambda) = \psi(\kappa) \langle \psi(\lambda) \mid \psi(q) \rangle, \]

where the index \( l \) labels the eigenfunctions of the one-dimensional Hamiltonian, and \( \langle q \mid \kappa \lambda \rangle \) is the distribution\textsuperscript{5}

\[ \langle q \mid \kappa \lambda \rangle = \left( \frac{\beta}{2\pi} \right)^{1/2} \sum_{m=-\infty}^{\infty} e^{i\phi_{\lambda m}} \delta(q - \lambda - m\rho). \]

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. \textsuperscript{4}.

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

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

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