A non-perturbative solution for Bloch electrons in constant magnetic fields

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A general theoretical approach for the non-perturbative Bloch solution of Schrödinger's equation in the presence of a constant magnetic field is presented. Using a singular gauge transformation based on a lattice of magnetic flux lines, an equivalent quantum system with a periodic vector potential is obtained. This system forms for rational magnetic fields a magnetic superlattice for which then Bloch's theorem applies. Extensions of the approach to particles with spin and many-body systems and connections to the theory of magnetic translation groups are discussed.

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The problem of electrons moving under the influence of a three-dimensional periodic potential and a tunable magnetic field is becoming an intriguing subject for physicists due to its remarkable complexity. Here we find a rich array of non-perturbative physics with predictions of fractal energy spectra - the famous Hofstadter butterfly [1], for which only very recently experimental evidence has been found in the quantized Hall conductance of superlattices [2]. At the same time, work on obtaining a satisfying theoretical description for these systems has been ongoing since many decades. The first analysis of Bloch electrons in a magnetic field dates back to Peierls [3] and is based on the tight-binding approximation. Within the envelope function approach, the standard method for introducing weak magnetic fields is the replacement of the wavevector in the $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian by an operator [4–9], a procedure that is sometimes called the Peierls substitution. But more recently it was shown that this approximation can lead to qualitatively incorrect results when the applied field introduces mixing between different energy bands [10]. And the question of integration path choice in tight-binding theory has lately become the matter of a vigorous debate [11–13]. Gauge invariant grid discretizations based on the Wilson formulation of lattice gauge theories [14] are more geared towards numerical purposes and do not explicitly exploit the periodicity of the crystal potential. And methods that express the crystal potential as a coupling matrix between Landau levels [15, 16] appear only feasible for very simple crystal potentials.

The reason for these difficulties lies directly in the non-existence of a Bloch solution for an electron moving in a periodic crystal potential $V(\mathbf{x})$ in the presence of a constant magnetic field $\mathbf{B}$

$$i\hbar\frac{\partial\Psi}{\partial t}=\frac{1}{2m}\left(\hat{\mathbf{p}}+e\mathbf{A}\right)^2\Psi+V\left(\mathbf{x}\right)\Psi, \qquad (1)$$

$$\mathbf{A}(\mathbf{x})=\frac{1}{2}\mathbf{B}\times\mathbf{x}+\text{gauge terms}. \qquad (2)$$

The vector potential $\mathbf{A}(\mathbf{x})$ is obviously not periodic here and cannot be made periodic for any gauge choice. Thus Bloch's theorem cannot be used to reduce (1) to the unit cell, and most of the standard methods in solid-state structure theory remain inaccessible. However, it is the goal of this Letter to show that by using a *singular* gauge transformation [17, 18] $\Psi=U(\mathbf{x})\psi$ it is possible to transform (1) into a new quantum system

$$i\hbar\frac{\partial\psi}{\partial t}=\frac{1}{2m}\left(\hat{\mathbf{p}}+e\mathbf{A}_p\right)^2\psi+V\left(\mathbf{x}\right)\psi, \qquad (3)$$

where the vector potential $\mathbf{A}_p\left(\mathbf{x}\right)$ is now periodic with a periodicity that is dependent on the magnetic field strength. For rational magnetic field strengths [19] the periodicities of $V\left(\mathbf{x}\right)$ and $\mathbf{A}_p\left(\mathbf{x}\right)$ will become commensurable, and we will obtain a magnetic superlattice where we can apply Bloch's theorem as

$$\psi\left(\mathbf{x}\right)=\mathrm{e}^{i\mathbf{k}\cdot\mathbf{x}}u_{\mathbf{k}}\left(\mathbf{x}\right) \qquad (4)$$

in order to obtain a reduced Schrödinger equation

$$i\hbar\frac{\partial u_{\mathbf{k}}}{\partial t}=\frac{1}{2m}\left(\hat{\mathbf{p}}+\hbar\mathbf{k}+e\mathbf{A}_p\right)^2u_{\mathbf{k}}+V\left(\mathbf{x}\right)u_{\mathbf{k}} \qquad (5)$$

for the magnetic unit cell. We will also show that the derivation demonstrated in this Letter is general enough to be generalized to particles with spin and the many-body case, and we will discuss connections to the theory of magnetic translation groups [20, 21].

In order to construct the singular gauge transform needed for obtaining (5), we start out by considering the physical properties of *magnetic flux lines*. In this context, we define a magnetic flux line as the limiting case of a magnetic flux tube with infinite length and infinitesimal thickness. For example, a flux line in the z-direction containing a flux Φ through the origin would be described by

$$\mathbf{B}\left(x,y,z\right)=\Phi\delta\left(x\right)\delta\left(y\right)\mathbf{e}_z=\Phi\delta_2\left(\mathbf{x}\right)\mathbf{e}_z, \qquad (6)$$

where δ_2 denotes the two-dimensional delta function and $\mathbf{e}_z$ the unit vector in the z-direction. It should be emphasized that in this paper we employ magnetic flux lines as a purely mathematical trick. We also do not imply any connections to the magnetic field lines commonly used to illustrate plots of magnetic fields. A suitable vector potential $\mathbf{A}_1$ describing this magnetic field is

$$\mathbf{A}_1\left(x,y\right)=\frac{\Phi}{2\pi\left(x^2+y^2\right)}\begin{pmatrix}-y\\ x\end{pmatrix}=\frac{\Phi}{2\pi\rho}\mathbf{e}_\varphi, \qquad (7)$$

where ρ and φ are the radial distance and the angle in cylindrical coordinates, and $\mathbf{e}_\varphi$ the unit vector in the φ-direction. Schrödinger's equation for this vector potential $\mathbf{A}_1$ and the vanishing crystal potential $V(\mathbf{x})$ contains the essence of the Aharonov-Bohm effect: An interference experiment with electrons around the flux line will result in a phase shift

$$\Delta = \frac{e}{\hbar c}\oint \mathbf{A}_1(\mathbf{x})\cdot \mathrm{d}\mathbf{x} = \frac{\Phi e}{\hbar} = \frac{2\pi\Phi}{\Phi_0}, \qquad (8)$$

where $\Phi_0 = h/e$ is the magnetic flux quantum. If the flux contained in the flux line is equal to Φ_0, the resulting phase shift becomes 2π and is therefore experimentally undetectable.

We now perform the transformation

$$\Psi(\rho,\varphi,z) = \exp(-i\varphi)\,\psi(\rho,\varphi,z) \qquad (9)$$

for the original Schrödinger equation (1). This transformation does not constitute a gauge transformation in the classical sense since the phase factor is not continuous at $\rho = 0$, even though transformations of the type (9) are sometimes called singular gauge transformations [17, 18]. Schrödinger's equation (1) now becomes

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(\hat{\mathbf{p}} + e\mathbf{A} - \frac{e\Phi_0}{2\pi\rho}\mathbf{e}_\varphi\right)^2\psi + V(\mathbf{x})\,\psi. \qquad (10)$$

Thus we have changed the original quantum problem (1) into a new one with a modified vector potential, where the extra term subtracted from $\mathbf{A}$ is the vector potential of a magnetic flux line through the origin with flux Φ_0 (7). It is clear that neither the probability density nor the energy spectrum is modified by the described procedure, which is straightforward to generalize to the case of multiple flux lines placed at different locations.

As next step, we examine an infinite lattice of identical parallel flux lines

$$\mathbf{B}(\mathbf{x}) = B_0\mathbf{e}_z - \Phi_0\sum_{\mathbf{x}_\mathrm{m}}\delta_2(\mathbf{x}-\mathbf{x}_\mathrm{m})\,\mathbf{e}_z, \qquad (11)$$

where Φ_0 is again the magnetic flux quantum, $\{\mathbf{x}_\mathrm{m}\}$ a two-dimensional point lattice in the x-y-plane

$$\mathbf{x}_\mathrm{m} = n_1\mathbf{c}_1 + n_2\mathbf{c}_2, \quad n_1, n_2 \text{ integer}, \qquad (12)$$

and $B_0\mathbf{e}_z$ a constant background magnetic field to set the average magnetic flux equal to zero

$$B_0 = \frac{\Phi_0}{|\mathbf{c}_1\times\mathbf{c}_2|} = \frac{\Phi_0}{S}, \qquad (13)$$

with S being the unit cell area. The vector potential $\mathbf{A}_p(x,y)$ belonging to this field can be found by making the ansatz

$$\mathbf{A}_p(x,y) = \mathbf{e}_z\times\nabla\chi(x,y) \qquad (14)$$

for the vector potential where $\chi(x,y)$ is a two-dimensional potential. We immediately find that

$$\nabla\times\mathbf{A}_p = \nabla^2\chi\mathbf{e}_z - \partial_z\nabla\chi = \nabla^2\chi\mathbf{e}_z. \qquad (15)$$

We now use that the magnetic field (11) is essentially two-dimensional $\mathbf{B}(x,y,z) = B(x,y)\,\mathbf{e}_z$, giving us together with the previous equation that the scalar potential χ is the solution of the two-dimensional Poisson equation

$$\left(\partial_x^2 + \partial_y^2\right)\chi(x,y) = B(x,y)\,. \qquad (16)$$

The solution of equation (16) is a two-dimensional Madelung problem. A very fast converging series for χ has been obtained in the context of the Ginzburg-Landau equations for the ideal Abrikosov vortex lattice in type-II superconductors [22]. Translating the result from [22] to our notation, we have

$$\chi(\mathbf{x}) = -\frac{\Phi_0}{4\pi}\log\left[\sum_{\mathbf{G}} a_\mathbf{G}\left(1-\cos\mathbf{G}\cdot\mathbf{x}\right)\right], \qquad (17)$$

$$a_\mathbf{G} = -(-1)^{n_1+n_2+n_1n_2}\exp\left(\frac{-SG^2}{8\pi}\right), \qquad (18)$$

with $\mathbf{G} = n_1\mathbf{d}_1 + n_2\mathbf{d}_2$ and $\mathbf{d}_1$,$\mathbf{d}_2$ being the reciprocal basis vectors of the flux line lattice. A corresponding periodic vector potential $\mathbf{A}_p$ can then be easily calculated via equation (14) using the gradient of the series (17).

Having obtained $\mathbf{A}_p$, we can construct a singular gauge transformation similar to (9) that adds a flux line lattice to the vector potential in Hamiltonian (1) such that the vector potential becomes periodic and Bloch's theorem becomes applicable. Denoting with $\mathbf{A}_F(\mathbf{x})$ the vector potential that describes a flux line lattice in the z-direction without a magnetic background field

$$\nabla\times\mathbf{A}_F(\mathbf{x}) = \mathbf{e}_z\sum_{\mathbf{x}_\mathrm{m}}\Phi_0\delta_2(\mathbf{x}-\mathbf{x}_\mathrm{m})\,, \qquad (19)$$

we now define a phase factor

$$U(\mathbf{x}) = \exp\left(-\frac{ie}{\hbar c}\int_\mathbf{0}^\mathbf{x}\mathbf{A}_F(\mathbf{x})\cdot\mathrm{d}\mathbf{x}\right). \qquad (20)$$

This phase factor is uniquely defined and therefore no explicit integration path for the integral needs to be specified. This crucial result can be easily shown if we consider that each flux line contains exactly one magnetic flux quantum Φ_0. Therefore due to Stokes' theorem changes in the integration path can only result in phase changes that are multiples of 2π. In addition, this uniqueness also gives us the important relationship

$$\nabla U(\mathbf{x}) = -\frac{ie}{\hbar}\mathbf{A}_F(\mathbf{x})\,U(\mathbf{x}). \qquad (21)$$

Next we choose a unit cell for the magnetic flux line lattice $\{\mathbf{c}_1,\mathbf{c}_2\}$ such that (13) holds (assuming $\mathbf{B} = B_0\mathbf{e}_z$ in equation (2) for simplicity) and that the average magnetic flux disappears . Using the singular gauge transformation

$$\Psi = U(\mathbf{x})\psi \qquad (22)$$

together with (21) we immediately get

$$i\hbar\frac{\partial\psi}{\partial t}=\frac{1}{2m}\left(\hat{\mathbf{p}}+e\mathbf{A}-e\mathbf{A}_F\right)^2\psi+V\left(\mathbf{x}\right)\psi. \quad (23)$$

But at the same time $\mathbf{A}_F$ is closely related to the previously calculated periodic vector potential $\mathbf{A}_p$ as

$$\mathbf{A}_p\left(\mathbf{x}\right)\equiv\frac{1}{2}\mathbf{B}\times\mathbf{x}-\mathbf{A}_F\left(\mathbf{x}\right)+\text{gauge terms.} \quad (24)$$

Therefore, ignoring gauge terms (which can be eliminated using an extra phase factor) we have made the vector potential periodic, giving us the final equation

$$i\hbar\frac{\partial\psi}{\partial t}=\frac{1}{2m}\left(\hat{\mathbf{p}}+e\mathbf{A}_p\right)^2\psi+V\left(\mathbf{x}\right)\psi. \quad (25)$$

Obviously we have now obtained a Hamiltonian for which both the crystal lattice in $V\left(\mathbf{x}\right)$ and the vector potential $\mathbf{A}_p\left(\mathbf{x}\right)$ are periodic. While the periodicity in $V\left(\mathbf{x}\right)$ is obviously fixed for a given material, the one of $\mathbf{A}_p\left(\mathbf{x}\right)$ is directly dependent on the applied magnetic field $\mathbf{B}$ due to equation (13). This has the consequence that for some magnetic field strengths the two periodicities can become commensurable and a magnetic superlattice forms. Specifically, we can obtain a magnetic superlattice if and only if we have a rational magnetic field as

$$\mathbf{B}\cdot\left(\mathbf{a}_i\times\mathbf{a}_j\right)=\epsilon_{ijk}\frac{p_k}{q_k}\Phi_0, \quad (26)$$

where $\mathbf{a}_1,\mathbf{a}_2,\mathbf{a}_3$ denotes a basis for the crystal lattice, ϵ_{ijk} the unit antisymmetric tensor, and p_k and q_k integers with no common factor. In this case we can construct a new unit cell for the crystal called the magnetic unit cell [19] such that $\mathbf{a}_3$ now points in the z-direction and

$$\mathbf{B}\cdot\left(\mathbf{a}_1\times\mathbf{a}_2\right)=n\Phi_0\,,\quad n\text{ integer,} \quad (27)$$

where $n=\pm 1$ for experimentally attainable field strengths. We now employ the remaining freedom in equation (13) for choosing the basis vectors of the magnetic flux line lattice by placing exactly one flux line in each magnetic unit cell (for $|n|>1$ we place $|n|$ flux lines into the magnetic unit cell instead), essentially selecting the projection of $\{\mathbf{a}_1,\mathbf{a}_2\}$ on the x-y-plane as the flux line basis $\{\mathbf{c}_1,\mathbf{c}_2\}$. We can then apply Bloch's theorem in order to obtain a reduced Schrödinger equation (5) within the magnetic unit cell. On the other hand, for irrational magnetic field strengths the periods of $V\left(\mathbf{x}\right)$ and $\mathbf{A}_p\left(\mathbf{x}\right)$ remain incommensurable and no magnetic superlattice with a finite unit cell can be constructed.

The derivation shown here will also go through in the presence of spin or a many-body Schrödinger equation. In the first case, we start with a Pauli-equation with spin-orbit coupling

$$i\hbar\frac{\partial\Psi}{\partial t}=\frac{1}{2m}\left[\left(\hat{\mathbf{p}}+e\mathbf{A}\right)\cdot\sigma\right]^2\Psi+V\left(\mathbf{x}\right)\Psi + V_{SO}\left[\mathbf{A}\right]\Psi, \quad (28)$$

$$V_{SO}\left[\mathbf{A}\right]=\frac{\hbar}{4m^2c^2}\sigma\cdot\nabla V(\mathbf{x})\times\left(\hat{\mathbf{p}}+e\mathbf{A}\right), \quad (29)$$

where Ψ is now a two-component spinor and σ the Pauli vector. We now define a singular gauge transformation

$$\Psi=U(\mathbf{x})\psi \quad (30)$$

using the same phase factor used previously (20). Since $U(\mathbf{x})$ commutes with σ, property (21) immediately gives us the expression

$$i\hbar\frac{\partial\psi}{\partial t}=\frac{1}{2m}\left[\left(\hat{\mathbf{p}}+e\mathbf{A}_p\right)\cdot\sigma\right]^2\psi+V\left(\mathbf{x}\right)\psi + V_{SO}\left[\mathbf{A}_p\right]\psi, \quad (31)$$

which again is a periodic system for rational magnetic fields. Similarly, for a many-body system

$$i\hbar\frac{\partial\Psi}{\partial t}=\left[\sum_{j=1}^{n}\frac{1}{2m_j}\left[\hat{\mathbf{p}}_j+e_j\mathbf{A}\left(\mathbf{x}_j\right)\right]^2+V\left(\mathbf{x}_j\right)\right]\Psi + V\left(\mathbf{x}_1,\ldots,\mathbf{x}_n\right)\Psi \quad (32)$$

we may use a transformation

$$\Psi(\mathbf{x}_1,\ldots,\mathbf{x}_n)=U_1(\mathbf{x}_1)\cdots U_n(\mathbf{x}_n)\psi(\mathbf{x}_1,\ldots,\mathbf{x}_n) \quad (33)$$

with n phase factors

$$U_j(\mathbf{x}_j)=\exp\left(-\frac{ie_j}{\hbar c}\int_{\mathbf{0}}^{\mathbf{x}_j}\mathbf{A}_F\left(\mathbf{x}\right)\cdot\mathrm{d}\mathbf{x}\right) \quad (34)$$

in order to obtain a periodic system

$$i\hbar\frac{\partial\psi}{\partial t}=\sum_{j=1}^{n}\left[\frac{1}{2m_j}\left[\hat{\mathbf{p}}_j+e_j\mathbf{A}_p\left(\mathbf{x}_j\right)\right]^2+V\left(\mathbf{x}_j\right)\right]\psi + V\left(\mathbf{x}_1,\ldots,\mathbf{x}_n\right)\psi. \quad (35)$$

However, in this case care has to be taken, since for different charges e_j the phase factors in (34) will remain multi-valued, unless all charges e_j are a multiple of the unit charge e. Of course, for an electronic system this is always the case.

An important question we still need to examine is how to compute matrix elements of observables. For observables that are only dependent on the position $O(\hat{\mathbf{x}})$, we find that its matrix elements remain unchanged

$$\left\langle\Psi_1\left|O(\hat{\mathbf{x}})\right|\Psi_2\right\rangle=\left\langle\psi_1\left|O(\hat{\mathbf{x}})\right|\psi_2\right\rangle. \quad (36)$$

For example, for the electric dipole $\mathbf{E}\cdot\hat{\mathbf{x}}$ this gives us for two eigenvectors Ψ_1,Ψ_2 with different energies E_1,E_2

$$\left\langle\Psi_1\left|\mathbf{E}\cdot\hat{\mathbf{x}}\right|\Psi_2\right\rangle=\frac{\left\langle\psi_1\left|\mathbf{E}\cdot\left(\hat{\mathbf{p}}+e\mathbf{A}_p\right)\right|\psi_2\right\rangle}{im\left(E_1-E_2\right)/\hbar}, \quad (37)$$

where we have inserted the commutator between the periodic Hamilton operator from equation (3) and the position operator $\hat{\mathbf{x}}$. On the other hand, for observables that are momentum-dependent $O(\hat{\mathbf{p}})$ we have to take property (21) into account which gives us

$$\left\langle\Psi_1\left|O(\hat{\mathbf{p}})\right|\Psi_2\right\rangle=\left\langle\psi_1\left|O(\hat{\mathbf{x}},\hat{\mathbf{p}}-e\mathbf{A}_F)\right|\psi_2\right\rangle. \quad (38)$$

We also get for observables $O(\hat{\mathbf{p}}+e\mathbf{A})$ the result

$$\langle \Psi_1 | O(\hat{\mathbf{p}}+e\mathbf{A}) | \Psi_2 \rangle = \langle \psi_1 | O(\hat{\mathbf{p}}+e\mathbf{A}_p) | \psi_2 \rangle . \tag{39}$$

Finally it is very interesting to examine the behavior of the phase factors (20) under translations. For any vector $\mathbf{c}$ in the flux line lattice we have the decomposition

$$U(\mathbf{x}+\mathbf{c}) = U(\mathbf{c}) \exp\left(-\frac{ie}{\hbar} \int_{\mathbf{c}}^{\mathbf{x}+\mathbf{c}} \mathbf{A}_F \cdot \mathrm{d}\mathbf{x} \right) \tag{40}$$

due to the path-independence of all integrals in (20). We then use (24) together with the periodicity of $\mathbf{A}_p$ to obtain the relationship

$$\mathbf{A}_F(\mathbf{x}+\mathbf{c}) - \mathbf{A}_F(\mathbf{x}) = \frac{1}{2}\mathbf{B}\times\mathbf{c}, \tag{41}$$

which we can use for shifting the integration path in (40) as

$$U(\mathbf{x}+\mathbf{c}) = U(\mathbf{c})U(\mathbf{x}) \exp\left(-\frac{ie}{2\hbar} \mathbf{B}\times\mathbf{x}\cdot\mathbf{c} \right) \tag{42}$$

or

$$\exp\left[\frac{i}{\hbar} \left(\hat{\mathbf{p}} + \frac{e}{2}\mathbf{B}\times\hat{\mathbf{x}} \right) \cdot \mathbf{c} \right] U(\mathbf{x}) = U(\mathbf{c})U(\mathbf{x}). \tag{43}$$

The exponential defined here is known as magnetic translation operator and can be used for a group-theoretical approach to the Bloch electron in a constant magnetic field [20, 21]. Therefore we have shown that the phase factor $U(\mathbf{x})$ is up to a gauge phase an eigenfunction of this operator for primitive translations of the magnetic flux line lattice.

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