The Wannier Functions of the Lattice Electron in a Uniform Magnetic Field

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In this paper a generalization of the WANNIER functions is performed for the case of the lattice electron moving in a uniform magnetic field.

In the case of the free electron moving in a uniform external magnetic field, the WANNIER function may be obtained directly by the Schrauben-function, if the wave vector $\boldsymbol{k}$ is substituted by the vector potential $-(1/c)\,\boldsymbol{A}(\boldsymbol{a}_j)$.

The WANNIER functions [1] introduced for the study of the properties of metals and generally the solid state, play a significant role in the theory of perturbation in metals.

The WANNIER functions $\alpha_n(\boldsymbol{r}-\boldsymbol{a}_q)$ are defined by the BLOCH [2] eigenfunctions $\Psi_{\boldsymbol{k},n}(\boldsymbol{r})$ and are related through a unitary transformation: i. e.

$$\alpha_n(\boldsymbol{r}-\boldsymbol{a}_q)=\frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}}\Psi_{\boldsymbol{k},n}(\boldsymbol{r}-\boldsymbol{a}_q) \tag{1}$$
$$=\frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}}\exp\{-i(\boldsymbol{k},\boldsymbol{a}_q)\}\cdot\Psi_{\boldsymbol{k},n}(\boldsymbol{r}),$$
$$\Psi_{\boldsymbol{k},n}(\boldsymbol{r})=\frac{1}{\sqrt{N}}\sum_{q}\exp\{i(\boldsymbol{k},\boldsymbol{a}_q)\}\cdot\alpha_n(\boldsymbol{r}-\boldsymbol{a}_q)$$

where N is the number of units cells and $\boldsymbol{a}_q$ is the lattice vector.

The above expression of the WANNIER functions has been taken from SCHNAKENBERG [3].

The WANNIER functions are orthogonal with respect to the position number q and the number n which characterises the energy bands.

The general properties of the WANNIER functions are treated in detail in the works of KOHN [4], BULYANITSA–SVETLOV [5] and EILENBERGER [6].

When an external magnetic field exists, then according to EILENBERGER [6] the new WANNIER functions are not orthogonal with respect to the position number q, but for weak fields they form a functional system which is independent and complete. It will be proven in the following that these hold for the case of the free electron moving in a uniform magnetic field as well.

We shall extend the definition of the WANNIER functions to the case of uniform external magnetic field.

$$\alpha_n(\boldsymbol{r}-\boldsymbol{a}_q,H)\sim\sum_{\boldsymbol{k}}\exp\{-i(\boldsymbol{k},\boldsymbol{a}_q)\}\cdot\Psi_{\boldsymbol{k},n}(\boldsymbol{r},H) \tag{2}$$

where $\Psi_{\boldsymbol{k},n}(\boldsymbol{r},H)$ is a solution of the following SCHRÖDINGER equation:

$$\left[-\frac{1}{2}\left(\nabla-\frac{i}{c}\boldsymbol{A}(\boldsymbol{r})\right)^2+V(\boldsymbol{r})-E_n(\boldsymbol{k})\right]\Psi_{\boldsymbol{k},n}(\boldsymbol{r},H)=0 \tag{3}$$

in atomic units $\hbar=1$, $m=1$, $e=1$. $\boldsymbol{A}(\boldsymbol{r})=\frac{1}{2}\boldsymbol{H}\times\boldsymbol{r}$ represents the vector potential, H is the magnetic field parallel to the z-axis, $V(\boldsymbol{r})$ is the lattice potential and $E_n(\boldsymbol{k})$ are the eigenvalues of energy.

In the Thesis of the author [7] the behavior of the lattice electron in a uniform external magnetic field has been treated by direct study of the SCHRÖDINGER equation (3). The proper eigenfunctions and the eigenvalues of the energy were obtained.

Now we shall determine the WANNIER functions for the case of a free electron as well as the lattice electron in uniform external magnetic field.

Wannier Function for Free Electron in Magnetic Field

For the free electron moving in a uniform magnetic field use is made of the Schraubenfunction [7]. The properties of which are more convenient than the eigenfunctions of LANDAU [8] and DINGLE [9].

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1 G. WANNIER, Phys. Rev. **52**, 191 [1937].
2 F. BLOCH, Z. Phys. **52**, 555 [1928].
3 J. SCHNAKENBERG, Z. Phys. **171**, 199 [1962].
4 W. KOHN, Phys. Rev. **115**, 809, 1460 [1960].
5 D. BULYANITSA and Y. SVETLOV, Soviet Phys.-Solid State **4**, 981 [1962].
6 G. EILENBERGER, Z. Phys. **175**, 445 [1963].
7 A. JANNUSSIS, Phys. Status Solidi **6**, 217 [1964].
8 L. LANDAU, Z. Phys. **64**, 629 [1930].
9 R. DINGLE, Proc. Roy. Soc. London **A 211**, 500 [1952].

The Schraubenfunction is:

$$\Psi_{\varkappa,n}(\boldsymbol{r},H)=\sqrt{\frac{B}{2\pi}\left(\frac{2}{B}\right)^n\frac{1}{n!}}\exp\left\{-\frac{1}{B}(\varkappa_x^2+\varkappa_y^2)+i(\boldsymbol{\varkappa},\boldsymbol{r})\right\}\cdot(-\varkappa_y-i\varkappa_x)^n \tag{4}$$

where

$$\boldsymbol{\varkappa}=\boldsymbol{k}-(1/c)\,\boldsymbol{A}(\boldsymbol{r})\quad\text{and}\quad B=H/c. \tag{5}$$

The eigenfunctions (4) for $B\to 0$, $n\to\infty$ and $B\,n\to$ const. turn out to be the eigenfunctions of a free electron.

The WANNIER function (2) for the eigenfunction (4) are written as follows:

$$a(\boldsymbol{r}-\boldsymbol{a}_q,H)\sim\sum_{\boldsymbol{k}}\exp\{-i(\boldsymbol{k},\boldsymbol{a}_q)\}\cdot\Psi_{\varkappa,n}(\boldsymbol{r},H). \tag{6}$$

The summation here can be substituted by an integral since the variable parameter $\boldsymbol{k}$ is continuous.

The calculation of the integral is carried out for two dimensions since in the dimension along the magnetic field the electron is free and the WANNIER function in this dimension has been calculated by WANNIER [1]. From condition (5) we obtain:

$$a_n(\boldsymbol{r}-\boldsymbol{a}_q)\sim\sqrt{\frac{B}{2\pi}\left(\frac{2}{B}\right)^n\frac{1}{n!}}\iint\exp\left\{-i\left(\boldsymbol{\varkappa}+\frac{1}{c}\boldsymbol{A}(\boldsymbol{r})\right)\boldsymbol{a}_q-\frac{1}{B}\left((\varkappa_x^2+\varkappa_y^2)\right)\right\}\cdot\exp\{i(\boldsymbol{\varkappa},\boldsymbol{r})\}\cdot(-\varkappa_y-i\varkappa_x)^n\mathrm{d}\varkappa_x\,\mathrm{d}\varkappa_y \tag{7}$$

$$=\sqrt{\frac{B}{2\pi}\left(\frac{B}{2}\right)^n\frac{1}{n!}}\exp\left\{-\frac{i}{c}\left(\boldsymbol{a}_q,\boldsymbol{A}(\boldsymbol{r})\right)-\frac{B}{4}\left[(x-q_1a_1)^2+(y-q_2a_2)^2\right]\right\}\left[(x-q_1a_1)+(y-q_2a_2)\right]^n$$

or

$$a_n(\boldsymbol{r}-\boldsymbol{a}_q,H)\sim\Psi_{-(1/c)\boldsymbol{A}(\boldsymbol{a}_q),n}(\boldsymbol{r}) \tag{8}$$

i. e. the WANNIER functions for free electron in uniform external magnetic field is a Schraubenfunction in two dimensions, the central point of which is $(q_1a_1,\ q_2a_2)$.

The above result, i. e. the WANNIER functions for the free electron moving in a uniform magnetic field may be obtained directly by the Schraubenfunction if the wave vector $\boldsymbol{k}$ is substituted by the vector potential $-(1/c)\boldsymbol{A}(\boldsymbol{a}_q)$. The WANNIER function (8) is therefore the solution of the SCHRÖDINGER equation (3) for the free electron in a uniform magnetic field.

The new WANNIER functions possess the following properties.

They satisfy the completeness condition and for different centers they are not orthogonal, i. e.

$$(a_n(\boldsymbol{r}-\boldsymbol{a}_q,H),a_m(\boldsymbol{r}-\boldsymbol{a}_g,H))=\exp\left\{-\frac{B}{4}\left[(\boldsymbol{a}_q-\boldsymbol{a}_g)^2+2\,i\,a_1a_2(g_1q_2-q_1g_2)\right]\right\}\delta_{nm},$$

$$(a_n(\boldsymbol{r}-\boldsymbol{a}_q,H),a_m(\boldsymbol{r}-\boldsymbol{a}_q,H))=\delta_{nm}. \tag{9}$$

Also the new WANNIER functions as the corresponding Schraubenfunctions (4) are localized and are of help for solving the SCHRÖDINGER equation (3) as was shown by the author [7].

Wannier Function for the Lattice Electron in Magnetic Field

The eigenfunctions of the lattice electron moving in a uniform magnetic field is a linear combination of Schraubenfunctions, of which the centers are the atoms of the lattice multiplied by a phase factor:

$$\Psi_{k,n}(\boldsymbol{r},H)=\sum_g\frac{\Phi^m_{g,n}(\boldsymbol{k})}{\sqrt{m!}}\exp\{2\pi i(\boldsymbol{r},\tilde{\boldsymbol{r}}_g)\}\cdot\Psi_{\varkappa,m}(\boldsymbol{r},H) \tag{10}$$

where $\Psi_{\varkappa,m}(\boldsymbol{r},H)$ is the Schraubenfunction for the free electron in a uniform magnetic field and $\tilde{\boldsymbol{r}}_g$ the reciprocal lattice vector.

The coefficients $\Phi^m_{g,n}(\boldsymbol{k})$ as well as the eigenvalues $E_n(\boldsymbol{k})$ of the energy are periodic functions of the vector $\boldsymbol{k}$ with period $(1/c)\,\boldsymbol{A}(\boldsymbol{a}_q)$.

According to HARPER [10] we can use $\boldsymbol{r}$ and $\boldsymbol{\varkappa}$ as independent variables and for constant $\boldsymbol{\varkappa}$ the eigenfunctions (10) will have the form of BLOCH [2] eigenfunctions.

In this case, the summation can be substituted by an integral since the variable parameter $\boldsymbol{k}$ is continuous. We obtain:

$$a_n(\boldsymbol{r}-\boldsymbol{a}_q, H) \sim \sum_{m=0}^{\infty} \frac{1}{\sqrt{m!}} \exp\{2\pi i(\boldsymbol{r}, \tilde{\boldsymbol{r}}_g)\} \cdot \int \mathrm{d}k \exp\{-i(\boldsymbol{k}, \boldsymbol{a}_q)\} \cdot \Phi_{g,n}^{m}(\boldsymbol{k})\, \Psi_{\boldsymbol{\varkappa},m}(\boldsymbol{r}, H). \tag{11}$$

In the case of a plane lattice potential it is possible to calculate the integral (11) if the following substitution is performed:

$$\Phi_{g,n}^{m}(\boldsymbol{k}) = F_{g,n}^{m} \exp\left\{-\frac{4\pi i}{B}\left(\frac{g_1}{a_1} k_y - \frac{g_2}{a_2} k_x\right)\right\}. \tag{12}$$

After the integration we obtain

$$a_n(\boldsymbol{r}-\boldsymbol{a}_q, H) \sim \sum_{g} \sum_{m=0}^{\infty} \frac{F_{g,n}^{m}}{\sqrt{m!}} a_m\left(\boldsymbol{r}-\boldsymbol{a}_q - \frac{4}{c B^2} \boldsymbol{A}(2\pi \tilde{\boldsymbol{r}}_g), H\right) \exp\{2\pi i(\boldsymbol{r}, \tilde{\boldsymbol{r}}_g)\} \tag{13}$$

where

$$a_m\left(\boldsymbol{r}-\boldsymbol{a}_q - \frac{4}{c B^2} \boldsymbol{A}(2\pi \tilde{\boldsymbol{r}}_g), H\right)$$

represents the WANNIER function for the free electron in a uniform magnetic field.

Consequently the WANNIER function for an electron moving in a uniform external magnetic field and plane lattice potential is a linear combination of WANNIER functions for the free electron in a uniform magnetic field multiplied by a phase factor.

[10] P. HARPER, Proc. Phys. Soc. London A **68**, 874, 879 [1955].