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PROPERTIES OF ELECTRON GAS IN CONSTANT MAGNETIC AND ELECTRIC FIELDS

Final Technical Report

by

Professor J. Zak

October 1977

EUROPEAN RESEARCH OFFICE

United States Army
London N.W.1, England
Contract Number DAERO 76-G-45

Technion Research and Development Foundation Ltd.
Technion - Israel Institute of Technology, Haifa, Israel

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20 Abstract

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Third, the symmetric coordinates in solids are used for developing Wannier functions in the presence of a magnetic field. The functions are shown to form an orthonormal set with respect to different bands and different sites of the crystal. A simple relation is established between the eigenfunctions of a Bloch electron in a magnetic field and the newly developed Wannier functions. This relation is used for an entirely elementary derivation of one-band effective Hamiltonians. Multiband operators are defined in the space of envelope functions for different physical quantities, e.g. the radius vector, velocity and acceleration.

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TABLE OF CONTENTS

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2. INTRODUCTION

The recent interest in the Koster-Slater impurity problem[1] was caused by a new idea put forward in a paper by Kohn and Onffroy[2]. The idea consists in defining one-band generalized Wannier functions (GWF) that are suitable for expanding the corresponding one-band eigenfunctions of a perturbed crystal. By doing so the multiband Koster-Slater equation reduces to a one-band problem. In addition, the local density of states and the charge density can directly be expressed in the GWF.

In this work an equation for defining localized states and effective Hamiltonians in perturbed crystals is developed. The equation is written in the framework of localized states in perfect crystals in the kq representation. The localization problem on ideal lattices[3,4] was recently solved and the approach here will be an extension of Ref. 4 to perturbed crystals. A variety of perturbations is considered, e.g. the impurity problem, the magnetic and electric fields. In developing the above-mentioned equation some simple facts about the localization problem in the kq-representation were used. First, a localized function in a perfect crystal, a Wannier function, for some band in the kq-representation is equal to the Bloch function for the same band. Secondly, localized functions in the kq-representation satisfy the Bloch equation for a perfect crystal. Thirdly, Wannier functions in the kq-representation for different sites differ from one another by a simple exponential factor. In a non-perfect crystal these facts can easily be generalized, and one is then lead to an equation for perturbed localized states. Because of their localized character, one expects the perturbed localized states not to differ very strongly from the corresponding localized states in a perfect crystal. Having this in mind, a pertubative procedure was developed in for deriving localized states and effective Hamiltonians in perturbed crystals.

Using the set of localized orthonormal functions a general theory is developed for deriving one-band effective Hamiltonians. The results are obtained up to second order in the perturbation expansion. The orthonormal functions that lead to the one-band effective Hamiltonians are shown to be suitable for deriving local charge densities in a crystal with a perturbation.

The perturbation expansion for the localized functions and the one-band effective Hamiltonian in this work is of quite general character and can be applied to a variety of problems, including the impurity problem, surfaces, superlattices and external fields[5-7]. The applicability of the approach is limited to crystals in which band touching does not appear and there is at least one isolated band. Good examples of this kind of crystals are the alkali halides, the rare gas solids and the II-VI semiconductor compounds.

The idea of using Wannier functions in the problem of a Bloch electron in a magnetic field was first given by Luttinger[8]. Later this idea was further developed for deriving effective one-band Hamiltonians in a paper by Roth[9].

The idea of modifying the Wannier functions in order to adjust them to the perturbation of a magnetic field is put forward in the Refs. (8) and (9). Following our perturbative approach, the Roth operator technique[9] is used for developing an orthonormal set of Wannier functions in the presence of a magnetic field. The newly defined Wannier functions are shown to be useful in deriving one-band effective Hamiltonians for a Bloch electron in a magnetic field in an entirely elementary way. These functions are also used to prove that the eigenfunction for a Bloch electron in a magnetic field can be written as a product of a known operator and the envelope function which satisfies the effective Hamiltonian equation. This structure of the eigenfunction serves as a basis for defining multiband operators in the space of the envelope functions for different physical quantities, e.g. the radius vector, the velocity, the acceleration, etc. Different relations are obtained between these operators fully resembling the corresponding relations in the absence of a magnetic field. In particular an acceleration theorem is proven to hold for the velocity of a Bloch electron in a magnetic field. It is also shown that a sum rule is satisfied by the newly defined operators[10].

3. EQUATION FOR LOCALIZED STATES IN PERTURBED CRYSTALS (REF. (6))

Let us start with a number of remarks about the kq representation and the problem of localized states in perfect crystals.

The connections between a wave function $\psi(\vec{r})$ in configuration space and the corresponding wave function $C(\vec{k},\vec{q})$ in the kq representation are as follows[11] :

$$\psi(\vec{r}) = \left(\frac{V_o}{(2\pi)^3}\right)^{1/2} \int d\vec{k}C(\vec{k},\vec{r}), \tag{1}$$

$$C(\vec{k},\vec{q}) = \left(\frac{V_o}{(2\pi)^3}\right)^{1/2} \sum_{\vec{R}} \exp(i\vec{k}\cdot\vec{R})\psi(\vec{q} - \vec{R}), \tag{2}$$

where V_o is the volume of a unit cell in the Bravais lattice, the integration in (1) is over the Brillouin zone, and the summation in (2) is over all the vectors $\vec{R}$ of the Bravais lattice. From (2) it follows that a Bloch function $C_{nk_B}(\vec{k},\vec{q})$ in the kq representation is

$$C_{nk_B}(\vec{k},\vec{q}) = \left(\frac{(2\pi)^3}{V_o}\right)^{1/2} \psi_{nk}(\vec{q})\sum_{\vec{K}} \delta(\vec{k} - \vec{k}_B - \vec{K}), \tag{3}$$

where $\psi_{nk}(\vec{q})$ is the Bloch function in the coordinate representation (with $\vec{r}$ replaced by $\vec{q}$), $\vec{k}_B$ is the Bloch quasimomentum, and the summation is over all the vectors $\vec{K}$ of the reciprocal lattice. By definition, a Wannier function $a'_{nm}(\vec{k},\vec{q})$ in the kq representation belonging to the nth band and located on site $\vec{R}_m$ of the Bravais lattice is

$$a'_{nm}(\vec{k},\vec{q}) = \left(\frac{V_o}{(2\pi)^3}\right)^{1/2} \int d\vec{k}_B \exp(-i\vec{k}_B\cdot\vec{R}_m)C_{nk_B}(\vec{k},\vec{q})$$

$$= \exp(-i\vec{k}\cdot\vec{R}_m)\psi_{nk}(\vec{q}) \qquad (4)$$

This is a very simple connection between a Wannier function in the kq representation and a Bloch function. The orthogonality of the Wannier functions (4) is seen immediately

$$\int d\vec{k}d\vec{q}\,a'^{*}_{nm}(\vec{k},\vec{q})a'_{n'm'}(\vec{k},\vec{q})$$

$$= \int \exp[i\vec{k}\cdot(\vec{R}_m - \vec{R}_{m'})]\psi^{*}_{nk}(\vec{q})\psi_{n'k}(\vec{q})d\vec{k}d\vec{q}$$

$$= \delta_{nn'}\delta_{mm'} \qquad (5)$$

For arriving at (5), we used the following relation that Bloch functions satisfy :

$$\frac{(2\pi)^3}{V_o}\int \psi^{*}_{nk}(\vec{q})\psi_{n'k}(\vec{q})d\vec{q} = \delta_{nn'} \qquad (6)$$

In what follows we shall prefer to work with the periodic part $U(\vec{k},\vec{q})$ of the wave function $C(\vec{k},\vec{q})$:

$$C(\vec{k},\vec{q}) = \exp(i\vec{k}\cdot\vec{q})U(\vec{k},\vec{q}), \tag{7}$$

where $U(\vec{k},\vec{q})$ is periodic in $\vec{q}$ with the period of a Bravais lattice vector $\vec{R}_n$ and Bloch periodic in $\vec{k}$,

$$U(\vec{k} + \vec{K}_m,\vec{q}) = \exp(-i\vec{q}\cdot\vec{K})U(\vec{k},\vec{q}),$$

with $\vec{K}_m$ a reciprocal-lattice vector. In an unperturbed crystal we have

$$\left(\frac{[-i(\partial/\partial\vec{q}) + \vec{k}]^2}{2m} + V(\vec{q})\right) U_{nk_B}(\vec{k},\vec{q}) = \varepsilon_n(\vec{k}_B)U_{nk_B}(\vec{k},\vec{q}) \tag{8}$$

where $U_{nk_B}(\vec{k},\vec{q})$ is the periodic part of the Bloch function in the kq representation

$$U_{nk_B}(\vec{k},\vec{q}) = \left(\frac{(2\pi)^3}{V_o}\right)^{1/2} u_{nk}(\vec{q}) \sum_{K_m} \delta(\vec{k} - \vec{k}_B - \vec{K}_m) \tag{9}$$

and $\varepsilon_n(\vec{k}_B)$ are the energy bands ($\vec{k}_B$ being the conserved quasimomentum). The periodic part of the Wannier functions $a_{nm}(\vec{k},\vec{q})$ is therefore

$$a_{nm}(\vec{k},\vec{q}) = \exp(-\vec{k}\cdot\vec{R}_m)u_{nk}(\vec{q}) \tag{10}$$

In what follows $a_{nm}(\vec{k},\vec{q})$ [and not the $a'_{nm}(\vec{k},\vec{q})$ in (4)] will be called the Wannier functions. It is obvious that the Wannier functions (10) satisfy in the kq representation the Bloch equation

$$\left(\frac{[-i(\partial/\partial\vec{q}) + \vec{k}]^2}{2m} + V(\vec{q})\right)a_{nm}(\vec{k},\vec{q}) = \varepsilon_n(\vec{k})a_{nm}(\vec{k},\vec{q}) \tag{11}$$

It is of interest to compare Eq. (8) for Bloch functions with Eq. (11) for Wannier functions. In Eq. (8), $\varepsilon_n(\vec{k}_B)$ is a constant independent of the kq coordinates while on the right-hand side of Eq. (11) we have $\varepsilon_n(\vec{k})$, a function of $\vec{k}$. We see that the only difference between the equation defining Bloch functions [Eq. (8)] and the equation defining localized functions [Eq. (11)] is in the factor multiplying the function on the right-hand side. This fact will be used in postulating an equation for localized states in perturbed crystals.

The Schrödinger equation for a Bloch electron in a constant magnetic field $\vec{H}$ and perturbation $v(\vec{r})$ in the kq representation is[11]

$$\left(\frac{[-i\partial/\partial\vec{q} + \vec{k} + (e/2c)\vec{H}\times i\partial/\partial\vec{k}]^2}{2m} + V(\vec{q}) + v\left(i\frac{\partial}{\partial\vec{k}}\right)\right) U(\vec{k},\vec{q}) =$$

$$= \varepsilon U(\vec{k},\vec{q}) \qquad (12)$$

Equation (12) is the eigenvalue equation (ε is a constant) for an electron in a perturbed crystal. The solutions $U(\vec{k},\vec{q})$ are eigenstates of the problem. In order to obtain an equation for localized states we shall use the analogy with equations (8) and (11). Equation (8) is an eigenstate equation [with a constant $\varepsilon_n(\vec{k}_B)$ multiplying the function on the right-hand side], while Eq. (11) defines localized states $a_{nm}(\vec{k},\vec{q})$ [the energy $\varepsilon_n(\vec{k})$ multiplies $a_{nm}(\vec{k},\vec{q})$ on the right-hand side]. Having this in mind we shall postulate in correspondence with Eq. (12) the following equation for localized functions in a perturbed crystal :

$$\left(\frac{[-i\partial/\partial\vec{q} + \vec{k} + (e/2c)\vec{H}\times i\partial/\partial\vec{k}]^2}{2m} + V(\vec{q}) \right.$$

$$\left. + v\left(i\frac{\partial}{\partial\vec{k}}\right)\right) A_{nm}(\vec{k},\vec{q}) = E_n(\vec{k},\vec{R}_m) A_{nm}(\vec{k},\vec{q}) \qquad (13)$$

where A_{nm} $(\vec{k},\vec{q})$ are the perturbed localized functions and $E_n(\vec{k},\vec{R}_m)$ are the effective band energies. The explicit dependence on the site $\vec{R}_m$ appears in the equation if one follows the structure of localized functions (10) in the kq-representation

$$A_{mn}(\vec{k},\vec{q}) - \exp(-i\vec{k}\cdot\vec{R}_m)U_{nm}(\vec{k},\vec{q}) \tag{14}$$

with $U_{nm}(\vec{k},\vec{q})$ satisfying the equation

$$\left(\frac{[-i\partial/\partial\vec{q} + \vec{k} + (e/2c)\vec{H}\times(\vec{R}_m + i\partial/\partial\vec{k})]^2}{2m} + V(\vec{q}) + v\left(i\frac{\partial}{\partial\vec{k}} + \vec{R}_m\right)\right) U_{nm}(\vec{k},\vec{q}) = E_n(\vec{k},\vec{R}_m)U_{nm}(\vec{k},\vec{q}) \tag{15}$$

In the absence of perturbations ($H = 0$, $v = 0$) Eq. (15) goes over into Eq. (11) for localized states of a perfect crystal. In the latter case the localized functions $U_{nm}(\vec{k},\vec{q})$ and the effective band energies $E_n(\vec{k},\vec{R}_m)$ are site $\vec{R}_m$ independent

$$U_{nm}(\vec{k},\vec{q}) = u_{nk}(\vec{q}) \tag{16}$$

$$E_n(\vec{k},\vec{R}_m) = \varepsilon_n(\vec{k}) \tag{17}$$

This is no longer so when a perturbation is present. As is seen from Eq. (15), both the localized functions $U_{nm}(\vec{k},\vec{q})$ and the effective band energies $E_n(\vec{k},\vec{R}_m)$ will, in general, be $\vec{R}_m$ dependent (an exception is the homogeneous electric field case). One should expect Eq. (15) to lead to localized states because the solution of the unperturbed equation [Eq. (11)] are localized and they should not be strongly affected by the perturbations. It is therefore possible, in principle, to solve

Eq. (15) by a perturbation procedure starting with the unperturbed equation (11). This is the main advantage of the localized equation (15) over the eigen-value equation (12). The eigenfunctions $U(\vec{k},\vec{q})$ of the latter are very different from the eigenfunctions $U_{nk_b}(\vec{k},\vec{q})$ of the unperturbed problem (8) and a perturbation procedure can, in general, not be applied to Eq. (12).

For comparison reasons let us write Eqs. (11) and (13) for localized states in the regular $\vec{r}$ representation. The left-hand sides of Eqs. (11) and (13) will just be the corresponding Hamiltonians applied to the function in the $\vec{r}$ representation. In order to obtain the right-hand side we expand the band energies $\varepsilon_n(\vec{k})$ and $E_n(\vec{k},\vec{R}_m)$ in Fourier series and use formula (1). Equations (11) and (13) in the $\vec{r}$ representation will be

$$\left(\frac{p^2}{2m} + V(\vec{r})\right) a_n(\vec{r} - \vec{R}_m) = \sum_s h_n(\vec{R}_s) a_n(\vec{r} - \vec{R}_m + \vec{R}_s),$$

$$\left(\frac{[\vec{p} + (e/2c)\vec{H}\times\vec{r}]^2}{2m} + V(\vec{r}) + v(\vec{r})\right) A_{nm}(\vec{r} - \vec{R}_m)$$

$$= \sum_s H_n(\vec{R}_s, \vec{R}_m) A_{nm}(\vec{r} - \vec{R}_m + \vec{R}_s), \qquad (19)$$

where

$$h_n(\vec{R}_s) = \frac{V_o}{(2\pi)^3} \int e^{-i\vec{k}\cdot\vec{R}_s} \varepsilon_n(\vec{k}) d\vec{k} \qquad (20)$$

$$H_n(\vec{R}_s, \vec{R}_m) = \frac{V_o}{(2\pi)^3} \int e^{-i\vec{k}\cdot\vec{R}_s} E_n(\vec{k},\vec{R}_m) d\vec{k} \qquad (21)$$

and $a_n(\vec{r} - \vec{R}_m)$, $A_{nm}(\vec{r} - \vec{R}_\ell)$ are the localized functions for the perfect and perturbed crystal, correspondingly. Equation (18) is well known and is the equation for Wannier functions $a_n(\vec{r})$ in a perfect crystal. In this case the shape of the function $a_n(\vec{r} - \vec{R}_m)$ does not vary with the site and all the Wannier functions for a given band are derived from a single function $a_n(\vec{r})$. In the perturbed crystal the shape of the localized function $A_{nm}(\vec{r} - \vec{R}_\ell)$ depends also on the site

$$A_{nm}(\vec{r} - \vec{R}_\ell) = \left(\frac{V_o}{(2\pi)^3}\right)^{1/2} \int d\vec{k}\, \exp(-i\vec{k}\cdot\vec{R}_\ell) C_{nm}(\vec{k},\vec{r}) \tag{22}$$

where $C_{nm}(\vec{k},\vec{r}) = \exp(i\vec{k}\cdot\vec{r}) U_{nm}(\vec{k},\vec{r})$ [see Eq. (1)]. In the regular r-representation, Eqs. (18) and (19) appear to be more complicated than Eqs. (11) and (13) and we find it more convenient to work in the kq representation.

4. THE IMPURITY PROBLEM

In the presence of an impurity perturbation v ($\vec{H} = 0$), Eq. (15) for localized states becomes

$$\left(\frac{(-i\partial/\partial\vec{q} + \vec{k})^2}{2m} + V(\vec{q}) + v\left(i\frac{\partial}{\partial\vec{k}} + \vec{R}_m\right)\right) U_{nm}(\vec{k},\vec{q})$$

$$= E_n(\vec{k},\vec{R}_m) U_{nm}(\vec{k},\vec{q}) \tag{23}$$

We shall solve Eq. (23) by a perturbation procedure assuming that the unperturbed bands $\varepsilon_n(\vec{k})$ are well separated. This will be needed for defining a parameter of smallness for the perturbation theory. Any function $U(\vec{k},\vec{q})$ can be expanded in the complete set of functions (10),

$$U(\vec{k},\vec{q}) = \sum_{nm} B_{nm} \exp(-i\vec{k}\cdot\vec{R}_m) u_{nk}(\vec{q})$$

$$= \sum_n B_n(\vec{k}) u_{nk}(\vec{q}) \tag{24}$$

which is a well known expansion in the kq representation[11]. For the solutions $U_{nm}(\vec{k},\vec{q})$ of Eq. (23), expansion (24) will be

$$U_{nm}(\vec{k},\vec{q}) = \sum_{\ell} B_{n\ell}(\vec{k},\vec{R}_m) u_{\ell k}(\vec{q}) \qquad (25)$$

In this case the expansion coefficients are site $\vec{R}_m$ dependent. We substitute expansion (25) into Eq. (23), multiply it by $u^*_{sk}(\vec{q})$ from the left, and integrate over $\vec{q}$. We arrive at the following equation for the coefficients $B_{nl}(\vec{k},\vec{R}_m)$:

$$\varepsilon_s(\vec{k}) B_{ns}(\vec{k},\vec{R}_m) + \sum_{\ell} v_{s\ell}\left(\vec{k}, i\frac{\partial}{\partial\vec{k}} + \vec{R}_m\right) B_{n\ell}(\vec{k},\vec{R}_m)$$

$$= E_n(\vec{k},\vec{R}_m) B_{ns}(\vec{k},\vec{R}_m), \qquad (26)$$

where

$$v_{s\ell}\left(\vec{k}, i\frac{\partial}{\partial\vec{k}} + \vec{R}_m\right) = \frac{(2\pi)^3}{V_o} \int u^*_{sk}(\vec{q}) v\left(i\frac{\partial}{\partial\vec{k}} + \vec{R}_m\right) u_{\ell k}(\vec{q}) d\vec{q} \qquad (27)$$

Expression (27) defines an operator which is to be applied to the coefficients $B_{n\ell}(\vec{k},\vec{R}_m)$, and the integrand from point of view of the quasimomentum $\vec{k}$ is a product of three operators. Equation (26) can be solved by perturbation theory. Let us introduce the following notations :

$$B_{ns}(\vec{k},\vec{R}_m) = B^{(0)}_{ns}(\vec{k},\vec{R}_m) + B^{(1)}_{ns}(\vec{k},\vec{R}_m) + B^{(2)}_{ns}(\vec{k},\vec{R}_m) + \ldots \qquad (28)$$

$$E_n(\vec{k},\vec{R}_m) = \varepsilon_n(\vec{k}) + \varepsilon^{(1)}_n(\vec{k},\vec{R}_m) + \varepsilon^{(2)}_n(\vec{k},\vec{R}_m) + \ldots \qquad (29)$$

where the superscript denotes the order of perturbation. Up to second order in the perturbation we have (we apply perturbation theory to band n)

$$B^{(0)}_{ns}(\vec{k},\vec{R}_m) = \delta_{ns} \tag{30}$$

$$B^{(1)}_{ns}(\vec{k},\vec{R}_m) = \frac{v_{sn}(\vec{k},\vec{R}_m)}{\varepsilon_n(\vec{k}) - \varepsilon_s(\vec{k})}, \quad s \neq n; \; B^{(1)}_{nn}(\vec{k},\vec{R}_m) = 0 \tag{31}$$

$$B^{(2)}_{ns}(\vec{k},\vec{R}_m) = \sum_{\ell \neq n} \frac{v_{s\ell}(\vec{k}, i\partial/\partial\vec{k} + \vec{R}_m) B^{(1)}_{n\ell}(\vec{k},\vec{R}_m)}{\varepsilon_n(\vec{k}) - \varepsilon_s(\vec{k})}$$

$$- \frac{v_{nn}(\vec{k},\vec{R}_m) v_{sn}(\vec{k},\vec{R}_m)}{[\varepsilon_n(\vec{k}) - \varepsilon_s(\vec{k})^2} \quad s \neq n \tag{32}$$

$$B^{(2)}_{nn\ell}(\vec{k},\vec{R}_m) = -\frac{1}{2} \sum_{\ell \neq n} \frac{v_{\ell n}(\vec{k},\vec{R}_m)^2}{[\varepsilon_n(\vec{k}) - \varepsilon_\ell(\vec{k})]^2} \tag{33}$$

$$\varepsilon^{(1)}_n(\vec{k},\vec{R}_m) = v_{nn}(\vec{k},\vec{R}_m), \tag{34}$$

$$\varepsilon^{(2)}_n(\vec{k},\vec{R}_m) = \sum_{\ell \neq n} v_{n\ell}\left(\vec{k}, i\frac{\partial}{\partial\vec{k}} + \vec{R}_m\right) B^{(1)}_{n\ell}(\vec{k},\vec{R}_m) \tag{35}$$

In the above formulas in addition to the matrix operator (27) also the matrix $v_{\ell s}(\vec{k},\vec{R}_m)$ appears. The latter is a special case of the operator (27) when it no longer operates on a function of $\vec{k}$ [the operator $v(i\partial/\partial\vec{k} + \vec{R}_m)$ in the integrand of (27) operates in this case directly on the function $u_{\ell k}(\vec{q})$]

$$v_{s\ell}(\vec{k},\vec{R}_m) = \sum_R \exp(-i\vec{k}\cdot\vec{R}) \times \ d\vec{r} a_s^*(\vec{r}-\vec{R}) v(\vec{r}+\vec{R}_m) a_\ell(\vec{r})$$

$$= \sum_R \exp(i\vec{k}\cdot\vec{R}) v_{s\ell}(\vec{R}_m+\vec{R},\vec{R}_m) \tag{36}$$

with

$$v_{s\ell}(\vec{R},\vec{R}') = \int a_s^*(\vec{r}-\vec{R}) v(\vec{r}) a_\ell(\vec{r}-\vec{R}') d\vec{r} \tag{37}$$

For results (30)-(35) to have the meaning of perturbation corrections we have to assume that

$$\eta = v_{sn}(\vec{k},\vec{R}_m)/[\varepsilon_n(\vec{k})-\varepsilon_s(\vec{k})] << 1, \tag{38}$$

where η is in some sense the expansion parameter of the perturbation theory.

When (38) holds the localized functions $A_{nm}(\vec{k},\vec{q})$ for a crystal with an impurity up to second order in perturbation theory will be

$$A_{nm}(\vec{k},\vec{q}) = \exp(-i\vec{k}\cdot\vec{R}_m) \times \Big([1 + B_{nn}^{(2)}(\vec{k},\vec{R}_m)] u_{nk}(\vec{q})$$

$$+ \sum_{s\neq n} [B_{ns}^{(1)}(\vec{k},\vec{R}_m) + B_{ns}^{(2)}(\vec{k},\vec{R}_m)] u_{sk}(\vec{q}) \Big) \tag{39}$$

where the coefficients $B_{ns}(\vec{k},\vec{R}_m)$ are given by (31)-(33).

The functions (39) by the construction of perturbation theory are normalized to second order in the perturbation

$$\int |A_{nm}(\vec{k},\vec{q})|^2 d\vec{k}d\vec{q} \approx 1 + B^{(2)}_{nn}(\vec{k},\vec{R}_m) + B^{(2)*}_{nn}(\vec{k},\vec{R}_m)$$

$$+ \sum_{s\neq n} |B^{(1)}_{ns}(\vec{k},\vec{R}_m)|^2 = 1 \qquad (40)$$

The last equality in (40) is a consequence of (31) and (33).

By using these results a one hand effective Hamiltonian can be derived for the impurity problem. The derivation will be based on the localized functions $A_{nm}(\overrightarrow{kq})$ [Eq. (39)] and the effective one band energies (39) and (35). Following some simple physical assumptions of Ref. (6), the localized functions $A_{nm}(\overrightarrow{kq})$ assume the following form to first order of the perturbation

$$A_{nm}(\vec{k},\vec{q}) = \exp(-i\vec{k}\cdot\vec{R}_m) \times \Big(u_{nk}(\vec{q}) +$$

$$\sum_{s\neq n} \frac{v_{ns}(\vec{R}_m)}{\varepsilon_{ns}} u_{sk}(\vec{q})\Big) \qquad (41)$$

The structure of the localized functions (41) is very simple and they can easily be written in the $\vec{r}$ representation

$$A_{nm}(\vec{r} - \vec{R}_m) = a_n(\vec{r} - \vec{R}_m) + \sum_{s\neq n} \frac{v_{ns}(\vec{R}_m)}{\varepsilon_{ns}} a_s(\vec{r} - \vec{R}_m) \qquad (42)$$

Here, $A_{nm}(\vec{r} - \vec{R}_m)$ are the localized functions for a crystal with an impurity. It is seen that $A_{nm}(\vec{r} - \vec{R}_m)$ depends not only on the difference $\vec{r} - \vec{R}_m$ as in the unperturbed Wannier functions $a_n(\vec{r} - \vec{R}_m)$ but also explicitly on the site $\vec{R}_m$. As should be expected, the stronger the perturbation is on site $\vec{R}_m$, the more will the perturbed function $A_{nm}(\vec{r} - \vec{R}_m)$ differ from the unperturbed one $a_n(\vec{r} - \vec{R}_m)$ on this particular site $\vec{R}_m$.

The assumptions simplify also considerably expressions (34) and (35) for the effective energies. To second order in perturbation theory we have

$$\varepsilon_n^{(1)}(\vec{k}, \vec{R}_m) = v_{nn}(\vec{R}_m) \;, \tag{43}$$

$$\varepsilon_n^{(2)}(\vec{k}, \vec{R}_m) = \sum_{s\neq n} \frac{|v_{ns}(\vec{R}_m)|^2}{\varepsilon_{ns}} \tag{44}$$

Let us now construct a one-band effective Hamiltonian for the impurity problem. For this purpose we expand the solution $U(\vec{k}, \vec{q})$ of Eq. (12) (with $\vec{H} = 0$) in the localized function $A_{\ell p}(\vec{k}, \vec{q})$,

$$U(\vec{k}, \vec{q}) = \sum_{\ell p} F_\ell(\vec{R}_p) A_{\ell p}(\vec{k}, \vec{q}), \tag{45}$$

where the expansion coefficients $F_\ell(\vec{R}_p)$ depend on the band index ℓ and the site $\vec{R}_m$. Substituting (45) into (12) we have

$$\sum_{\ell p} E_\ell(\vec{k}, \vec{R}_p) F_\ell(\vec{R}_p) A_{\ell p}(\vec{k}, \vec{q}) = \varepsilon \sum_{\ell p} F_\ell(\vec{R}_p) A_{\ell p}(\vec{k}, \vec{q}) \;, \tag{46}$$

where

$$E_\ell(\vec{k}, \vec{R}_p) = \varepsilon_\ell(\vec{k}) + v_\ell\,(\vec{R}_p) + \sum_{s\neq \ell} \frac{|v_{\ell s}(\vec{R}_p)|^2}{\varepsilon_{\ell s}} \;. \tag{47}$$

Up to the order of η^2 the one-band effective Hamiltonian equation for the impurity problem will be

$$\sum_p h_n(\vec{R}_p - \vec{R}_m) F_n(\vec{R}_p)$$

$$+ \Big(v_{nn}(\vec{R}_m) + \sum_{s\neq n} \frac{|v_{ns}(\vec{R}_m)|^2}{\varepsilon_{ns}}\Big) F_n(\vec{R}_m) = \varepsilon F_n(\vec{R}_m) \;. \tag{48}$$

Equation (49) has a correction term

$$\sum_{s\neq n} \frac{|v_{ns}(\vec{R}_m)|^2}{\varepsilon_{ns}}$$

to the well-known one-band classical equations for localized impurities of Koster and Slater[1] and for shallow impurities in the effective-mass approximation. Equation (48) reproduces both mentioned equations when the correction term is neglected. However, the second-order perturbation term in Eq. (48) is of very simple structure and can lead to significant contributions in the one band impurity potential. The significance of this term follows from the fact that while being a one-band band term it is influenced by the explicit band structure of the solid. This can in particular be easily seen in solving the Koster-Slater localized impurity problem. Thus by assuming that only two bands interact in Eq. (48) (band s influences band n) and that the impurity is localized at the origin, we find that the effective impurity potential at $\vec{R}_m = 0$ is

$$V_{nn}(0) + |v_{ns}(0)|^2/\varepsilon_{ns} \, . \tag{49}$$

This potential depends explicitly on the band gap ε_{ns} and the interband matrix elements $v_{ns}(0)$. The second-order correction term in (49) can be large and is restricted only by the applicability of perturbation theory. Both the binding energies of the impurity and scattering cross sections will be modified by the band structure.

Similar remarks can, in principle, be made about the significance of the correction term in Eq. (48) for the shallow impurity. In this case, however, one should, in general, expect that for gentle potentials $v(\vec{r})$ the second order term in (48) will be very small. One could, however, imagine cases when $v_{s\ell}(\vec{R})$ is not negligibly small. This is only a guess and it should be checked on real problems.

5. BLOCH ELECTRONS IN A MAGNETIC FIELD (REF . (10))

In the presence of a homogeneous magnetic field H the equation for localized states becomes

$$\left[\frac{(-i \frac{\partial}{\partial \vec{q}} + \vec{k} + \frac{e}{2c} \vec{H} \times i \frac{\partial}{\partial \vec{k}})^2}{2m} + V(\vec{q}) \right] A_{nm}(\vec{k}\vec{q}) = E_n(\vec{k},\vec{R}_m) \, A_{nm}(\vec{k}\vec{q}) \tag{50}$$

where $A_{nm}(\vec{k}\vec{q})$ is the perturbed localized function for band n and site R_m and $E_n(\vec{k},\vec{R}_m)$ is the site dependent effective energy. In the absence of the magnetic field, Eq. (50) goes over into Eq. (11) and correspondingly $A_{nm}(\vec{k}\vec{q})$ go into $a_{nm}(\vec{k}\vec{q})$ (Rel. (10)) and the $E_n(\vec{k},\vec{R}_m)$ become the unperturbed energies $\varepsilon_n(\vec{k})$. One can look for $A_{nm}(\vec{k}\vec{q})$ in the form

$$A_{nm}(\vec{k}\vec{q}) = \exp(-i\vec{k}\cdot\vec{R}_m)\ U_{nm}(\vec{k}\vec{q}) \tag{51}$$

where $U_{nm}(\vec{k}\vec{q})$ satisfies the equation[5]

$$\left[\frac{(-i\frac{\partial}{\partial\vec{q}} + \vec{k} + \frac{e}{2c}\vec{H}\times\vec{R}_m + \frac{e}{2c}\vec{H}\times i\frac{\partial}{\partial\vec{k}})^2}{} + V(\vec{q})\right] U_{nm}(\vec{k}\vec{q})$$

$$= E_n(\vec{k},\vec{R}_m)\ U_{nm}(\vec{k}\vec{q}) \tag{52}$$

The Hamiltonian in (52) depends on the combination

$$\vec{k}_m = \vec{k} + \frac{e}{2c}\vec{H}\times\vec{R}_m \tag{53}$$

which means that (51) can be rewritten as

$$A_{nm}(\vec{k}\vec{q}) = \exp(-i\vec{k}\cdot\vec{R}_m)\ U_{nk_m}(\vec{q}) \tag{54}$$

and $E_n(\vec{k},\vec{R}_m)$ in (52) will be

$$E_n(\vec{k},\vec{R}_m) = E_n(\vec{k}_m) \tag{55}$$

The results (50) - (54) can be written in a more compact form by using the notation $A(\vec{\chi})$ for a function of the operator $\vec{\chi} = \vec{k} + \frac{e}{2c}\vec{H}\times i\frac{\partial}{\partial\vec{k}}$. $A(\vec{\chi})$ is defined as follows

$$A(\vec{\chi}) = \int d\vec{\lambda}\ F(\vec{\lambda})\ \exp\{i(\vec{k} + \frac{e}{2c}\vec{H}\times i\frac{\partial}{\partial\vec{k}})\cdot\vec{\lambda}\} \tag{56}$$

where $F(\vec{\lambda})$ is the Fourier transform of $A(\vec{k})$. In Ref. (9) a simple multiplication rule was shown to hold for a product of two operators

$$A(\vec{\chi})\ B(\vec{\chi}) = C(\vec{\chi}) \tag{57}$$

where

$$C(\vec{k}) = A(\vec{k})\ B(\vec{k}) = ih_{\alpha\beta}\ \frac{\partial A(\vec{k})}{\partial k_{\alpha}}\ \frac{\partial B(\vec{k})}{\partial k_{\beta}} - $$

$$- \frac{1}{2}\ h_{\alpha\beta}\ h_{\alpha'\beta'}\ \frac{\partial^2 A(\vec{k})}{\partial k_{\alpha}\partial k_{\alpha'}}\ \frac{\partial^2 B(\vec{k})}{\partial k_{\beta}\partial k_{\beta'}} + \dots \tag{58}$$

and

$$h_{\alpha\beta} = \varepsilon_{\alpha\beta\gamma}\ \frac{eH_{\gamma}}{2c} \tag{59}$$

In (59) $\varepsilon_{\alpha\beta\gamma}$ is the antisymmetric unit tensor and in (58) and (59) there are summations over repeated indices. Rel. (57) together with (58) and (59) give what is called the commutator expansion in powers of the magnetic for a product of two functions of $\vec{\chi}$.

By using notation (58) the localized functions (54) can be written as follows:

$$A_{nm}(\vec{k}\vec{q}) = U_n(\vec{\chi}\vec{q})\ \exp(-i\vec{k}\cdot\vec{R}_m) \tag{60}$$

where $U_n(\vec{\chi}\vec{q})$ operates on $\exp(-i\vec{k}\cdot\vec{R}_m)$. Similarly, Eq. (50) can be rewritten as

$$H(\vec{\chi}\vec{q})\ U_n(\vec{\chi}\vec{q})\ \exp(-i\vec{k}\cdot\vec{R}_m) = (E_n(\vec{k})\ U_n(\vec{k}\vec{q}))_{\vec{k}=\vec{\chi}}\ \exp(-i\vec{k}\cdot\vec{R}_m) \tag{61}$$

where $H(\vec{k}\vec{q})$ is the Bloch Hamiltonian. On both sides of Eq. (61) there are operators which are applied to the function $\exp(-i\vec{k}\cdot\vec{R}_m)$. Without the latter Eq. (61) is an operator equation. For reasons that will become clear below it is convenient to write this operator equation in a somewhat different form

$$H(\vec{\chi}\vec{q})\ U_n(\vec{\chi}\vec{q}) = U_n(\vec{\chi}\vec{q})\ H_n(\vec{\chi}) \tag{62}$$

On the right hand side of Eq. (62) the operators are rearranged in comparison with Eq. (61) and this is the reason for writing $H_n(\vec{k})$ instead of $E_n(\vec{k})$. Eq. (62) will be the main equation for defining Wannier functions and one-band effective Hamiltonians for a Bloch electron in a magnetic field.

One can now prove that the functions $A_{nm}(\vec{k}\vec{q})$ in (60) are the Wannier functions of the problem.

Before turning to the solution of Eq. (62) let us show its connection with the eigenvalue problem for a Bloch electron in a magnetic field. The Schrödinger equation for the latter in the kq-representation can be written as follows

$$H(\vec{\chi}\vec{q})\; U(\vec{k}\vec{q}) = \varepsilon\; U(\vec{k}\vec{q}) \tag{63}$$

where $H(\vec{k}\vec{q})$ is the Hamiltonian and $H(\vec{\chi}\vec{q})$ is obtained from $H(\vec{k}\vec{q})$ by replacing in it $\vec{k}$ by $\vec{k} + \frac{e}{2c}\vec{H}\times i\frac{\partial}{\partial \vec{k}}$. It can be assumed that the Wannier functions $A_{nm}(\vec{k}\vec{q})$ in (61) form a complete set and the following expansion holds for the eigenfunction $U(\vec{k}\vec{q})$

$$U(\vec{k}\vec{q}) = \sum_{nm} F_n(\vec{R}_m)\; A_{nm}(\vec{k}\vec{q}) = \sum_n U_n(\vec{\chi}\vec{q})\; B_n(\vec{k}) \tag{64}$$

where $B_n(\vec{k})$ and $F_n(\vec{R}_m)$ are Fourier transforms of one another. Let us substitute Exp. (64) and (63) and use Eq. (62). We find

$$\sum_n U_n(\vec{\chi}\vec{q})\; H_n(\vec{\chi})\; B_n(\vec{k}) = \varepsilon \sum_n U_n(\vec{\chi}\vec{q})\; B_n(\vec{k}) \tag{65}$$

By multiplying Eq. (65) by $U_\ell^\dagger(\vec{\chi}\vec{q})$ from the left, and by integrating it over $\vec{q}$ one finds

$$H_\ell(\vec{\chi})\; B_\ell(\vec{k}) = \varepsilon\; B_\ell(\vec{k}) \tag{66}$$

which is a one-band effective Hamiltonian equation for a Bloch electron in a magnetic field. Eq. (66) shows that $H(\vec{k})$ in the equation for localized states (Eq. (62)) is the effective Hamiltonian of the problem. This means that by knowing the solutions of Eq. (62) one knows directly the one-band effective Hamiltonian. In addition, from Eq. (66) together with Exp. (64) one can find the eigenfunctions for a Bloch electron in a magnetic field. Since the operators $U_n(\vec{\chi}\vec{q})$ diagonalize the Hamiltonian, only one term should be kept in the Exp. (64) and the eigenfunction $U(\vec{k}\vec{q})$ corresponding to the band n becomes

$$U(\vec{k}\vec{q}) = U_n(\vec{\chi}\vec{q})\ B_n(\vec{k}) \tag{67}$$

In the kq-representation the eigenfunction $U(\vec{k}\vec{q})$ exhibits therefore a separation of the envelope function $B_n(\vec{k})$ and the crystalline operator $U_n(\vec{\chi}\vec{q})$. Rel. (67) shows that in the kq-representation the separation of the eigenfunction into a product of a known crystalline operator and an envelope function is a general one band feature without any additional assumptions. This general feature of the kq-representation is a consequence of the fact that k and q are the symmetric coordinates in an ideal crystal.

The solutions of the main equation (Eq. (62)) can be found as a power series of the magnetic field in the framework of the commutator expansion (57) - (59). It was already shown that these solutions give the one band effective Hamiltonian and the Wannier functions in the presence of a magnetic field. For solving Eq. (62) multiply it by $U_\ell^\dagger(\vec{\chi}\vec{q})$ from the left and integrate over $\vec{q}$

$$\frac{V_o}{(2\pi)^3} H_{\ell n}(\vec{\chi}) = \int U_\ell(\vec{\chi}\vec{q})\ H(\vec{\chi}\vec{q})\ U_n(\vec{\chi}\vec{q})d\vec{q} = \delta_{\ell n} \frac{V_o}{(2\pi)^3} H_n(\vec{\chi}) \tag{68}$$

The next step is to expand the function $U_n(\vec{k}\vec{q})$ in Wannier functions of the ideal crystal

$$U_n(\vec{k}\vec{q}) = \sum_s B_{ns}(\vec{k})\ u_{sk}(\vec{q}) \tag{69}$$

The unknowns are now the effective Hamiltonian $H_n(\vec{k})$ and the coefficients $B_{ns}(\vec{k})$. One can look for them in the form of a perturbation series

$$H_n(\vec{k}) = \varepsilon_n^{(o)}(\vec{k}) + \varepsilon_n^{(1)}(\vec{k}) + \varepsilon_n^{(2)}(\vec{k}) + \ldots \tag{70}$$

$$B_{ns}(\vec{k}) = \delta_{ns} + B_{ns}^{(1)}(\vec{k}) + B_{ns}^{(2)}(\vec{k}) + \ldots \tag{71}$$

where the superscripts denote different orders in the magnetic field according to the commutator expansion (57) - (59). It can be shown (Ref. (10)) that the effective Hamiltonian (Rel. (70)) and the coefficients (Rel. (71)) can be determined to any order of the magnetic field from Eq. (68) together with the orthogonality relation. By solving these equations it is shown with what ease one can reproduce the well known results of constructing one-band Hamiltonians for a Bloch electron without the need of using diagonalization procedures, Thus, the zero order effective Hamiltonian is

$$\varepsilon_n^{(o)}(\vec{k}) = \varepsilon_n(\vec{k}) \tag{72}$$

while the first order results are

$$\varepsilon_n^{(1)}(\vec{k}) = V_{nn}^{(1)}(\vec{k}) \tag{73}$$

$$B_{nn}^{(1)}(\vec{k}) = -\frac{1}{2} N_{nn}^{(1)}(\vec{k}) \tag{74}$$

while for $\ell \neq n$ one finds

$$B_{n\ell}^{(1)}(\vec{k}) = \frac{V_{\ell n}^{(1)}(\vec{k})}{\varepsilon_n(\vec{k}) - \varepsilon_\ell(\vec{k})} \tag{75}$$

The effective Hamiltonian (73) is identical with the one given by Formula (73) of Ref. (9). It is interesting that both the effective Hamiltonian (Ref. (73)) and the coefficient (Rel. (75)) to the first order in the magnetic field are determined by a unique non-Hermitian matrix. The expressions (73) and (75) look like first order perturbation formulas.

With the same ease one finds the second order terms in (70) and (71) (see Ref. (10)):

$$\varepsilon_n^{(2)}(\vec{k}) = G_{nn}^{(2)}(\vec{k}) - \varepsilon_n(\vec{k})\, N_{nn}^{(2)}(\vec{k}) + \sum_{s\neq n} \frac{|V_{sn}^{(1)}(\vec{k})|^2}{\varepsilon_n(\vec{k}) - \varepsilon_s(\vec{k})} - N_{nn}^{(1)}(\vec{k})\, V_{nn}^{(1)}(\vec{k}) \tag{76}$$

$$B_{nn}^{(2)}(\vec{k}) = -\frac{1}{2}\{N_{nn}^{(2)}(\vec{k}) + {}_{s}|B_{ns}^{(1)}(\vec{k})|^{2} + h_{\alpha\beta}\frac{\partial}{\partial k_{\beta}}\sum_{s}(B_{ns}^{(1)}(\vec{k})\,X_{\alpha ns}(\vec{k}) + \text{h.c.}) \tag{77}$$

By using the latter expressions one can show that the effective Hamiltonian $\varepsilon_{n}^{(2)}(\vec{k})$ in (76) is identical with the one given by Formula (74) of Ref. (9).

Similarly, for $\ell \neq n$ we have

$$\begin{aligned} B_{n\ell}^{(2)}(\vec{k}) = & \frac{1}{\varepsilon_{n}(\vec{k}) - \varepsilon_{\ell}(\vec{k})}\{G_{\ell n}^{(2)}(\vec{k}) - \varepsilon_{n}(\vec{k})\,N_{\ell n}^{(2)}(\vec{k}) + \\ & + \sum_{s} B_{\ell s}^{(1)*}(\vec{k})\,B_{ns}^{(1)}(\vec{k})\,(\varepsilon_{\ell}(\vec{k}) - \varepsilon_{s}(\vec{k})) + (B_{n\ell}^{(1)}(\vec{k})\,V_{\ell\ell}^{(1)}(\vec{k}) + \text{h.c.}) + \\ & + H_{\alpha\beta}\frac{\partial}{\partial k_{\alpha}}(i\,B_{n\ell}^{(1)}(\vec{k})\,v_{\beta\ell\ell}(\vec{k}) + \text{h.c.}) + h_{\alpha\beta}\frac{\partial}{\partial k_{\alpha}}\sum_{s} B_{ns}^{(1)}(\vec{k})\,X_{\beta\ell s}(\vec{k}) \end{aligned} \tag{78}$$

It is therefore seen that with very little algebra one finds from the Eq. (44) both the effective one-band Hamiltonian and the coefficients $B_{n\ell}(k)$. The latter determine the Wannier functions in a magnetic field (Rels. (61) and (69)). Thus, to the zero order of the magnetic field one has $(B_{n\ell}^{(o)} - \delta_{n\ell})$

$$A_{nm}(\vec{k}\vec{q}) = u_{nk_{m}}(\vec{q})\exp(-i\vec{k}\cdot\vec{R}_{m}) \tag{79}$$

where $\vec{k}_{m}$ is given in (53). The zero order Wannier functions in the presence of a magnetic field (Rel. (79)) are very similar to the corresponding functions in an ideal crystal. The former are obtained from the latter by replacing $\vec{k}$ in the periodic function $u_{nk}(q)$ by $\vec{k}_{m}$. The functions (79) are modified Wannier functions for the magnetic field problem and they were already used for describing the motion of a Bloch electron in a magnetic field.[8,9] Similarly, one obtains the Wannier functions to higher order, of the magnetic field.

In summary, the use of localized functions that correspond to nonideal crystals enables one to take directly into account multiband effects in the impurity problem and in the problem of external fields. Wannier functions in ideal crystals have been known as an extremely useful tool in general theoretical proofs and model calculations in solid state physics. The work reviewed in this report shows that a similar role is played by perturbation adapted localized functions in imperfect crystals.

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