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Derivation of Single-Band Effective Hamiltonian

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An alternative rigorous derivation is given of the operator equation on which the effective-mass theory for electrons in periodic potentials and applied fields is based. The relationship of this work to previous derivations is briefly discussed.

A simple derivation of the single-band effective Hamiltonian for electrons in a periodic potential, with applied electric and magnetic fields, has been given recently by Zak, [1] utilizing a representation based on eigenfunctions of a momentum space translation operator. In this "*kq* representation," $\vec{q}$ is a spatial variable which is conjugate to the reciprocal-lattice momentum vectors $\vec{K}_m$, and which ranges over a unit cell.

In view of the current interest in this approach, [2] it may be worth noting that an equally simple derivation of the single-band effective Hamiltonian may be obtained by using a representation based on relabeling the exponential functions $e^{i\vec{k}\cdot\vec{r}}$ which, as is already well known, form a complete set. For example, the operator equation from which the effective Hamiltonian is obtained[3,4] may be derived in a single step.

We observe that if for some particular lattice, $\vec{k}$ ranges over the first Brillouin zone in wave-vector space, and $\vec{K}_m$ ranges over all possible vectors of the reciprocal lattice, then the values of $\vec{k}+\vec{K}_m$ cover the entirety of wave-vector space and the set of functions $V^{-1/2}e^{i(\vec{k}+\vec{K}_m)\cdot\vec{r}}$ is complete. Here, V is the volume within which the functions are normalized. These functions, in the language of group theory, may be considered to be eigenfunctions of the group of commuting translation operators $e^{i(\vec{R}_n+\vec{g})\cdot\vec{p}/\hbar}$, where $\vec{R}_n$ is a lattice vector and $\vec{g}$ an arbitrary translation lying within a primitive unit cell.

We may then expand an arbitrary wave function $\psi(\vec{r})$ in terms of this set;

$$\vec{\psi}(\vec{r})=\left(\frac{V}{(2\pi)^3}\right)^{1/2}\sum_{\vec{K}_m}\int d^3k\exp[i(\vec{k}+\vec{K}_m)\cdot\vec{r}]D_{\vec{k},\vec{K}_m}\ , \tag{1}$$

where $D_{\vec{k},\vec{K}_m}$ is the wave function in the "$\vec{k}\vec{K}_m$ representation." It is evident that $D_{\vec{k},\vec{K}_m}$ is a function of the sum $\vec{k}+\vec{K}_m$, so that, for example,

$$D_{-1/2\,\vec{K}_i,\vec{K}_m+\vec{K}_i}=D_{1/2\,\vec{K}_i,\vec{K}_m}\ . \tag{2}$$

It is easily established that the momentum operator $\vec{p}$ in the $\vec{k}\vec{K}_m$ representation takes the form

$$p_{\vec{k},\vec{K}_m}=\hbar(\vec{k}+\vec{K}_m)\ . \tag{3}$$

The corresponding form of the position operator $\vec{r}$ is obtained as follows:

$$\vec{r}\psi(\vec{r})=\left(\frac{V}{(2\pi)^3}\right)^{1/2}\times\sum_{\vec{K}_m}\int d^3k\left(\frac{1}{i}\nabla_{\vec{k}}e^{i(\vec{k}+\vec{K}_m)\cdot\vec{r}}\right)D_{\vec{k},\vec{K}_m}\ . \tag{4}$$

Upon integrating by parts, the operator $i\nabla_{\vec{k}}$ is ap-

plied to $D_{\vec{k},\vec{K}_m}$. The boundary terms are a sum of surface integrals over the surface of the first Brillouin zone;

$$\sum_{\vec{K}_m} \int d^3k\, \nabla_{\vec{k}} [e^{i(\vec{k}+\vec{K}_m)\cdot\vec{r}}\, D_{\vec{k},\vec{K}_m}]$$

$$= \sum_{\vec{K}_m} \sum_{[(1/2)\vec{K}_i]} \int d\vec{S}_i\, e^{i(\vec{k}+\vec{K}_m)\cdot\vec{r}} D_{\vec{k},\vec{K}_m},$$

where $d\vec{S}_i$ is an outward normal over that part of the surface of the first Brillouin zone bounded by the plane which perpendicularly bisects the reciprocal-lattice vector $\vec{K}_i$. It is clear that, because of the property (2), the boundary term for a given $\vec{K}_m$ and $\frac{1}{2}\vec{K}_i$ will cancel with that corresponding to $\vec{K}_m+\vec{K}_i$ and $-\frac{1}{2}\vec{K}_i$. Hence all boundary contributions vanish, and

$$\vec{r}_{\vec{k},\vec{K}_m} = i\nabla_{\vec{k}}. \tag{5}$$

Since the potential $V(\vec{r})$ has the periodicity of the lattice, it can be expanded in a Fourier series

$$V(\vec{r}) = \sum_{\vec{K}_m} V(\vec{K}_m) e^{i\vec{K}_m\cdot\vec{r}}. \tag{6}$$

Then it may be shown that

$$V(\vec{r})\psi(\vec{r}) = \left(\frac{V}{(2\pi)^3}\right)^{1/2} \sum_{\vec{K}_m} \int d^3k \times e^{i(\vec{k}+\vec{K}_m)\cdot\vec{r}} \left\{ \sum_{\vec{K}_n} V(\vec{K}_m - \vec{K}_n) D_{\vec{k},\vec{K}_n} \right\}. \tag{7}$$

For constant applied magnetic and electric fields, the scalar and vector potentials for one choice of gauge take the following form:

$$\Phi_{\vec{k},\vec{K}_m} = -i\vec{E}\cdot\nabla_{\vec{k}}, \tag{8}$$

$$A_{\vec{k},\vec{K}_m} = \tfrac{1}{2} i \vec{H}\times\nabla_{\vec{k}}. \tag{9}$$

The single-particle Schrödinger equation in the $\vec{k}\vec{K}_m$ representation is then

$$\sum_{\vec{K}_n} H_{\vec{K}_m\vec{K}_n} D_{\vec{k},\vec{K}_n} = E D_{\vec{k},\vec{K}_m}, \tag{10}$$

where the Hamiltonian operator $H_{\vec{K}_m\vec{K}_n}$ is given by

$$H_{\vec{K}_m\vec{K}_n}(\vec{k}) = \frac{1}{2m}\left(\hbar(\vec{k}+\vec{K}_m) - \frac{ie}{2c}\vec{H}\times\nabla_{\vec{k}}\right)^2 \delta_{\vec{K}_m\vec{K}_n} + V(\vec{K}_m - \vec{K}_n) - ie\,\vec{E}\cdot\nabla_{\vec{k}}\delta_{\vec{K}_m\vec{K}_n}. \tag{11}$$

The operator equation (10) is equivalent to that obtained by Praddaude,[4] Blount,[5] and Zak.[1]

In order to demonstrate the utility of the present simple approach and to show its equivalence to the work of Zak, let us show how an effective one-band Hamiltonian can be obtained in this representation. We first write the Schrödinger equation in the $\vec{k}\vec{K}_m$ representation for zero fields. We use the notation $d^n_{\vec{k},\vec{K}_m}$ for the wave function, where the superscript n is a band index:

$$\frac{\hbar^2}{2m}(\vec{k}+\vec{K}_m)^2 d^n_{\vec{k},\vec{K}_m} + \sum_{\vec{K}_l} V(\vec{K}_m - \vec{K}_l)\, d^n_{\vec{k},\vec{K}_l} = E^n_{\vec{k}} d^n_{\vec{k},\vec{K}_m}. \tag{12}$$

In particular for $\vec{k}=0$,

$$\frac{\hbar^2}{2m}\vec{K}_m^2 d^n_{0,\vec{K}_m} + \sum_{\vec{K}_l} V(\vec{K}_m - \vec{K}_l)\, d^n_{0,\vec{K}_l} = E^n_0 d^n_{0,\vec{K}_m}. \tag{13}$$

Since different values of $\vec{k}$ are not coupled by Eq. (12), the energy eigenfunctions can be chosen to be Bloch functions, so that there is no sum over $\vec{k}$ in Eq. (1). Then for each value of $\vec{k}$, the wave functions $d^n_{\vec{k},\vec{K}_m}$ are solutions of a system of linear equations with constant coefficients, and obey the orthogonality and completeness relations

$$\sum_{\vec{K}_m} d^{n*}_{\vec{k},\vec{K}_m} d^m_{\vec{k},\vec{K}_m} = \delta_{nm}, \tag{14}$$

$$\sum_n d^{n*}_{\vec{k},\vec{K}_m} d^n_{\vec{k},\vec{K}_l} = \delta_{\vec{K}_m\vec{K}_l}. \tag{15}$$

Now consider a general solution $D_{\vec{k},\vec{K}_m}$ with fields on. We can construct an expansion of $D_{\vec{k},\vec{K}_m}$ in terms of $d^n_{\vec{k},\vec{K}_m}$ using the completeness relation for an arbitrary $\vec{k}'$;

$$D_{\vec{k},\vec{K}_m} = \left(\sum_n \sum_{\vec{K}_l} D_{\vec{k},\vec{K}_l} d^{n*}_{\vec{k}',\vec{K}_l}\right) d^n_{\vec{k}',\vec{K}_m}. \tag{16}$$

In particular if $\vec{k}'=0$, we introduce the coefficients $A_n(\vec{k})$ by means of

$$D_{\vec{k},\vec{K}_m} = \sum_n A_n(\vec{k}) d^n_{0,\vec{K}_m} \tag{17}$$

and if $\vec{k}'=\vec{k}$, the corresponding coefficients $B_n(\vec{k})$ are given by

$$D_{\vec{k},\vec{K}_m} = \sum_n B_n(\vec{k})\, d^n_{\vec{k},\vec{K}_m}. \tag{18}$$

Then from Eq. (16), the coefficients $A_n(\vec{k})$ and $B_n(\vec{k})$ are related by

$$A_n(\vec{k}) = \sum_j S_{nj}(\vec{k}) B_j(\vec{k}), \tag{19}$$

where

$$S_{nj}(\vec{k}) = \sum_{\vec{K}_l} d^{n*}_{0,\vec{K}_l} d^j_{\vec{k},\vec{K}_l}. \tag{20}$$

The matrix S is unitary, for it is easily verified from Eqs. (14) and (15) that

$$(S^\dagger S)_{nl} = \sum_{j,\vec{K}_m,\vec{K}_l} d^j_{0,\vec{K}_m} d^{n*}_{\vec{k},\vec{K}_m} d^{l*}_{0,\vec{K}_l} d^l_{\vec{k},\vec{K}_l} = \delta_{nl}. \tag{21}$$

Then using the expansion of $D_{\vec{k},\vec{K}_m}$ in terms of $d^n_{0,\vec{K}_m}$, together with Eq. (19),

$$D_{\vec{k},\vec{K}_m} = \sum_{n,j} S_{nj}(\vec{k}) B_j(\vec{k}) d^n_{0,\vec{K}_m} \tag{22}$$

and we have

$$\sum_{n,\vec{K}_l} H_{\vec{K}_m\vec{K}_l}(\vec{k}) \sum_j S_{nj}(\vec{k}) B_j(\vec{k}) d^n_{0,\vec{K}_l} = E_{\vec{k}} \sum_{n,j} S_{nj}(\vec{k}) d^n_{0,\vec{K}_m}. \tag{23}$$

After multiplying on the left by $d^{i}_{\vec{k},\vec{K}_m}$ and summing over all $\vec{K}_m$, the above equation reduces to

$$\sum_j (S^\dagger HS)_{ij} B_j(\vec{k}) = E_{\vec{k}} B_i(\vec{k}) , \tag{24}$$

where the matrix H_{in} appearing in Eq. (24) is given by

$$H_{in} = \sum_{\vec{K}_m,\vec{K}_l} d^{i*}_{0,\vec{K}_m} H_{\vec{K}_m,\vec{K}_l} d^{n}_{0,\vec{K}_l}, \tag{25}$$

the rows and columns of H_{in} being labeled by band indices.

It should be emphasized that the matrix S_{nj} defined in Eq. (20) in terms of a sum over reciprocal-lattice vectors is numerically *identical* to the matrix S_{nj} obtained by Zak[1] using the kq representation. S_{nj} in no way depends on the particular choice of kq or $k\vec{K}_m$ representations.

The single-band part of the Hamiltonian H_{in} may be separated out with the help of the definitions:

$$V_{in} = \sum_{\vec{K}_m,\vec{K}_l} d^{i*}_{0,\vec{K}_m} V(\vec{K}_m - \vec{K}_l) d^{n}_{0,\vec{K}_l} , \tag{26}$$

$$\vec{P}_{in} = \sum_{\vec{K}_m} d^{i*}_{0,\vec{K}_m} \hbar\vec{K}_m d^{n}_{0,\vec{K}_m} . \tag{27}$$

Then

$$H_{in} = \delta_{in}\left[\left(\frac{1}{2m}\right)\left(\hbar\vec{k} - \frac{ie}{2c} H\times\nabla_{\vec{k}}\right)^2 - ie\vec{E}\cdot\nabla_{\vec{k}}\right]$$

$$+ \sum_{\vec{K}_m,\vec{K}_l} d^{i*}_{0,\vec{K}_m}\left(\frac{\hbar^2 K_m^2}{2m}\delta_{\vec{K}_m\vec{K}_l} + V(\vec{K}_m - \vec{K}_l)\right) d^{n}_{0,\vec{K}_l}$$

$$+ \vec{P}_{in}\cdot\left(\hbar\vec{k} - \frac{ie}{2c}\vec{H}\times\nabla_{\vec{k}}\right)\Big/ m , \tag{28}$$

and using Eqs. (13) and (14)

$$H_{in} = \delta_{in}\left[\frac{1}{2m}\left(\hbar\vec{k} - \frac{ie}{2c} H\times\nabla_{\vec{k}}\right)^2 - ieE\cdot\nabla_{\vec{k}} + E^{i}_{0}\right]$$

$$+ \vec{P}_{in}\cdot\left(\hbar\vec{k} - \frac{ie}{2c} H\times\nabla_{\vec{k}}\right)\Big/ m. \tag{29}$$

A single-band effective Hamiltonian may be obtained by transforming away the interband terms in Eq. (29). In the absence of external fields, this can be accomplished by means of the matrix S defined in Eq. (20), for in this case it is easily verified that

$$(S^\dagger HS)_{ij} = E^{i}_{\vec{k}}\delta_{ij} . \tag{30}$$

With nonzero fields, an appropriately symmetrized matrix $[S_{in}(\vec{k})]$ may be used, as discussed by Roth[6] and Zak.[1] Acceleration theorems may also be proved using the symmetrized S; the calculations in the $\vec{k}\vec{K}_m$ representation are, however, identical to those in the kq representation, inasmuch as the matrix S does not depend on which representation is chosen.

[1]J. Zak, Phys. Rev. Letters 19, 1385 (1967); Phys. Rev. 168, 686 (1968).
[2]Phys. Today 22, 64 (1969); J. Zak, *ibid.* 23, 51 (1970).
[3]W. Kohn, Phys. Rev. 115, 1460 (1959).
[4]H. C. Praddaude, Phys. Rev. 140, A1292 (1965).
[5]E. I. Blount, Phys. Rev. 126, 1636 (1962).
[6]L. M. Roth, J. Phys. Chem. Solids 23, 433 (1962).

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Application of Gutzwiller's Variational Method to the Metal-Insulator Transition

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It is shown that the approximate variational calculation of Gutzwiller predicts a metal-insulator transition as the intra-atomic Coulomb interaction is increased for the case of one electron per atom. The susceptibility and effective mass are calculated in the metallic phase and are found to be enhanced by a common factor which diverges at the critical value of the interaction.

Several years ago, Gutzwiller[1] performed an approximate variational calculation of the ground-state wave function for a model Hamiltonian with a single tight-binding band and with only intra-atomic Coulomb interactions between the electrons. This model Hamiltonian, introduced earlier by Hubbard,[2] Gutzwiller,[3] and Kanamori,[4] is generally known as the Hubbard model and has been studied by many authors. Using Gutzwiller's[1] notation, as we shall in this paper, the model Hamiltonian has the form

$$H = \sum_{\vec{k}} \epsilon_{\vec{k}} (a^\dagger_{\vec{k}\uparrow} a_{\vec{k}\uparrow} + a^\dagger_{\vec{k}\downarrow} a_{\vec{k}\downarrow}) + C\sum_{\vec{g}} a^\dagger_{\vec{g}\uparrow} a^\dagger_{\vec{g}\downarrow} a_{\vec{g}\downarrow} a_{\vec{g}\uparrow} , \tag{1}$$

where $a^\dagger_{\vec{k}}$ and $a^\dagger_{\vec{g}}$ are the creation operators for elec-