

Bloch wave function in quantum Boltzmann equation

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There are several ways to build QBE in a crystal:

1. The most naive way is to insert the band structure $\epsilon_{n\mathbf{k}}$ into the LHS of QBE: thus we get corrected velocity. The main problem of this approach is it ignores the influence of the Bloch wave function; since the eigenstates in the crystal are no longer plane waves, defining a distribution function about \mathbf{r} and \mathbf{k} can't be done by naively doing Wigner transform.
2. One way to improve the situation is to start from the so-called Bloch semi-classic EOM about \mathbf{r} and \mathbf{k} ; we insert $\dot{\mathbf{r}}$ and $\dot{\mathbf{k}}$ given by the Bloch equations into the LHS of QBE.
This level of approximation is equivalent to building the QBE based on the effective Hamiltonian about the wave packet envelope. However, it doesn't include the effects of the Bloch wave functions to the collision term.
3. How to incorporate the effects of the Bloch wave functions into the collision term? Some kind of "wave packet envelope" seems to be needed, or otherwise gradient expansion is ill-defined; should we work in this basis (mapping Bloch state to plane waves, etc.)?
4. Further questions: hopping between bands (how frequent are they? Do we need $f_{n_1 n_2}(\mathbf{r}, \mathbf{k}, t)$? etc.)

1 Describing the wave packet in one band

In this section we ignore Coulomb scattering. Also, below we consider wave packet in one band first; the band index n is therefore fixed and not summed over.

1.1 No electric field coupling

Suppose we have a wave packet

$$\psi(\mathbf{r}, t) = \sum_{\mathbf{k}} c_{\mathbf{k}}(t) \psi_{n\mathbf{k}}(\mathbf{r}) = \sum_{\mathbf{k}} c_{\mathbf{k}}(t) u_{n\mathbf{k}}(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}}. \quad (1)$$

We consider the information of the spatial structure of ψ within a primitive unit cell as unimportant; in other words, we consider Fourier components with the wave vector being outside the 1BZ as unimportant. This filtering means the envelope of the wave packet is

$$\psi^{\text{envelope}}(\mathbf{r}, t) = \sum_{\mathbf{k}} c_{\mathbf{k}}(t) e^{i\mathbf{k} \cdot \mathbf{r}}, \quad (2)$$

where formally we set $u_{n\mathbf{k}}$ to unity.

We first deal with the case with no external driving electric field. In this case the total Hamiltonian is just the band Hamiltonian, and we have

$$i\partial_t \psi = H\psi \Rightarrow i\partial_t c_{\mathbf{k}} = \epsilon_{n\mathbf{k}} c_{\mathbf{k}} \Rightarrow i\partial_t \psi^{\text{envelope}} = \epsilon_{n\mathbf{k}}(\mathbf{k} \rightarrow -i\nabla) \psi^{\text{envelope}}. \quad (3)$$

The last line can be proved by properties of Fourier transform. Thus the effective Hamiltonian of the envelope function can be obtained by replacing \mathbf{k} with $-i\nabla$ in the band energy $\epsilon_{n\mathbf{k}}$. Thus, we conclude that when scattering is not considered and the effects of the external driving field is small, the naive approach of treating \mathbf{k} as the real momentum and replacing $\mathbf{k}^2/2m$ by $\epsilon_{n\mathbf{k}}$ is accurate enough.

1.2 Electric field coupling

When we do have electric field coupling things are different, since the coupling term $e\mathbf{r} \cdot \mathbf{E}$ ¹ doesn't necessarily appear to be the same in the effective Hamiltonian of the wave packets. The Schrodinger equation now is

$$i\partial_t\psi = H^{\text{band}}\psi + e\mathbf{r} \cdot \mathbf{E}\psi \Rightarrow i\partial_t c_{\mathbf{k}} = \varepsilon_{n\mathbf{k}} c_{\mathbf{k}} + \sum_{\mathbf{k}'} e\mathbf{E} \cdot \langle \psi_{n\mathbf{k}} | \mathbf{r} | \psi_{n\mathbf{k}'} \rangle c_{\mathbf{k}'}, \quad (5)$$

where we have assumed that \mathbf{E} changes slowly enough so it can be extracted out of the expectation brackets; this condition is needed for Boltzmann transportation anyway, or otherwise gradient expansion fails. The second term in the RHS of the second equation is notorious for being ill-defined: searching for a sensible definition of this term gave rise to the theory of band topology. To make things easier at the first step, let's do decomposition

$$\mathbf{r} \rightarrow \mathbf{r}^{\text{envelope}} + \mathbf{x}, \quad (6)$$

where $\mathbf{r}^{\text{envelope}}$ is the center of the wave packet. So we have

$$\sum_{\mathbf{k}'} e\mathbf{E} \cdot \langle \psi_{n\mathbf{k}} | \mathbf{r} | \psi_{n\mathbf{k}'} \rangle c_{\mathbf{k}'} = e\mathbf{E} \cdot \mathbf{r}^{\text{envelope}} c_{\mathbf{k}} + \sum_{\mathbf{k}'} e\mathbf{E} \cdot \langle \psi_{n\mathbf{k}} | \mathbf{x} | \psi_{n\mathbf{k}'} \rangle c_{\mathbf{k}'}, \quad (7)$$

where only the first term is non-zero in the free electron case. Since the \mathbf{x} term vanishes in a free electron gas, we can evaluate this term using the same techniques used when establishing relation between polarization and Berry curvature. We also change the normalization convention so that

$$\psi_{n\mathbf{k}} = \frac{1}{\sqrt{N}} e^{i\mathbf{k} \cdot \mathbf{r}} u_{n\mathbf{k}}. \quad (8)$$

We have

$$\begin{aligned} \langle \psi_{n\mathbf{k}} | \mathbf{x} | \psi_{n\mathbf{k}'} \rangle &= \frac{1}{N} \sum_{\mathbf{R}} \int_{\text{u.c.}} d^d \mathbf{x} e^{-i\mathbf{k} \cdot (\mathbf{x} + \mathbf{R})} u_{n\mathbf{k}}^*(\mathbf{x}) \cdot (\mathbf{x} + \mathbf{R}) \cdot e^{i\mathbf{k}' \cdot (\mathbf{x} + \mathbf{R})} u_{n\mathbf{k}'}(\mathbf{x}) \\ &= \frac{1}{N} \sum_{\mathbf{R}} e^{i\mathbf{R} \cdot (\mathbf{k}' - \mathbf{k})} \int_{\text{u.c.}} d^d \mathbf{x} e^{-i\mathbf{k} \cdot \mathbf{x}} u_{n\mathbf{k}}^*(\mathbf{x}) \cdot (\mathbf{x} + \mathbf{R}) \cdot e^{i\mathbf{k}' \cdot \mathbf{x}} u_{n\mathbf{k}'}(\mathbf{x}). \end{aligned} \quad (9)$$

The first line is obtained by expanding \mathbf{x} into $\mathbf{x} + \mathbf{R}$, where \mathbf{x} is confined in the primitive unit cell. The integral over \mathbf{x} can be split into one term with an \mathbf{x} factor and another with \mathbf{R} . The \mathbf{R} term has to vanish TODO: why?

The \mathbf{x} part in (9) is therefore the only non-zero part, and it reads

$$\begin{aligned} \langle \psi_{n\mathbf{k}} | \mathbf{x} | \psi_{n\mathbf{k}'} \rangle &= \delta_{\mathbf{k}\mathbf{k}'} \int_{\text{u.c.}} d^d \mathbf{x} e^{-i\mathbf{k} \cdot \mathbf{x}} u_{n\mathbf{k}}^*(\mathbf{x}) u_{n\mathbf{k}'}(\mathbf{x}) \cdot (-i\partial_{\mathbf{k}'}) e^{i\mathbf{k}' \cdot \mathbf{x}} \\ &= \delta_{\mathbf{k}\mathbf{k}'} \int_{\text{u.c.}} d^d \mathbf{x} e^{-i\mathbf{k} \cdot \mathbf{x}} u_{n\mathbf{k}}^*(\mathbf{x}) \cdot (-i\partial_{\mathbf{k}'}) u_{n\mathbf{k}'}(\mathbf{x}) e^{i\mathbf{k}' \cdot \mathbf{x}} \\ &\quad + \delta_{\mathbf{k}\mathbf{k}'} \int_{\text{u.c.}} d^d \mathbf{x} e^{-i\mathbf{k} \cdot \mathbf{x}} u_{n\mathbf{k}}^*(\mathbf{x}) \cdot e^{i\mathbf{k}' \cdot \mathbf{x}} (i\partial_{\mathbf{k}'}) u_{n\mathbf{k}'}(\mathbf{x}) \\ &= \delta_{\mathbf{k}\mathbf{k}'} (-i\partial_{\mathbf{k}'}) \int_{\text{u.c.}} d^d \mathbf{x} e^{-i\mathbf{k} \cdot \mathbf{x}} u_{n\mathbf{k}}^*(\mathbf{x}) \cdot u_{n\mathbf{k}'}(\mathbf{x}) e^{i\mathbf{k}' \cdot \mathbf{x}} \\ &\quad + \delta_{\mathbf{k}\mathbf{k}'} \int_{\text{u.c.}} d^d \mathbf{x} u_{n\mathbf{k}}^*(\mathbf{x}) \cdot (i\partial_{\mathbf{k}}) u_{n\mathbf{k}}(\mathbf{x}). \end{aligned} \quad (10)$$

The first term may be non-zero, but it vanishes once placed in a sum over \mathbf{k}' : we have

$$\sum_{\mathbf{k}'} c_{\mathbf{k}'} \delta_{\mathbf{k}\mathbf{k}'} (-i\partial_{\mathbf{k}'}) \int_{\text{u.c.}} d^d \mathbf{x} e^{-i\mathbf{k} \cdot \mathbf{x}} u_{n\mathbf{k}}^*(\mathbf{x}) \cdot u_{n\mathbf{k}'}(\mathbf{x}) e^{i\mathbf{k}' \cdot \mathbf{x}}$$

¹Here the convention is $e > 0$, and thus

$$q\varphi \approx q\mathbf{r} \cdot \nabla\varphi = -q\mathbf{r} \cdot \mathbf{E} = e\mathbf{r} \cdot \mathbf{E}. \quad (4)$$

TODO

The final conclusion is we have

$$i\partial_t c_{\mathbf{k}} = \varepsilon_{n\mathbf{k}} c_{\mathbf{k}} + e\mathbf{E} \cdot (\mathbf{r}^{\text{envelope}} + A_{n\mathbf{k}}), \quad A_{n\mathbf{k}} = i \langle u_{n\mathbf{k}} | \partial_{\mathbf{k}} | u_{n\mathbf{k}} \rangle, \quad (11)$$

and the effective Hamiltonian is now

$$H^{\text{envelope}} = (\varepsilon_{n\mathbf{k}} + e(\mathbf{r}^{\text{envelope}} + A_{n\mathbf{k}}) \cdot \mathbf{E})|_{\mathbf{k} \rightarrow -\nabla}. \quad (12)$$

This agrees with the effective Hamiltonian obtained from path integral formalism; in the latter, however, we don't know if the "position" variable is indeed the center of the wave packet, while here we explicitly show that the center of the wave packet does look like a position variable in quantum mechanics. Here we also replace the "real" position operator in \mathbf{E} by the center of wave packet, but since we have assumed that \mathbf{E} changes slowly enough, this substitution costs us almost nothing.

Note that the above derivation can also be seen as evaluating $\langle \psi_{n\mathbf{k}} | H | \psi_{n\mathbf{k}'} \rangle$, where the appearance of \mathbf{r} or in other words $i\partial_{\mathbf{k}}$ means different \mathbf{k} modes are mixed together by the dipole interaction term.