Bound on the group velocity of an electron in a one-dimensional periodic potential

Michael R. Geller and Giovanni Vignale
Institute for Theoretical Physics, University of California, Santa Barbara, Santa Barbara, California 93106
*and Department of Physics, University of Missouri, Columbia, Missouri 65211**
(Received 24 August 1994)

By using a recently derived upper bound on the allowed equilibrium current in a ring, it is proved that the magnitude of the group velocity of a Bloch electron in a one-dimensional periodic potential is always less than or equal to the group velocity of the same Bloch state in an empty lattice. Our inequality also implies that each energy band in a one-dimensional crystal always lies below the corresponding free-electron band, when the minima of those bands are aligned.

In a recent study,[1] one of us has shown that the equilibrium orbital current I flowing through a cross section of a toroidal body cannot exceed the fundamental limit

$$I_{\max}=\frac{Ne\hbar}{4\pi m r_0^2}\ , \tag{1}$$

where N is the total number of electrons, m is the free-electron mass, e is the magnitude of the electron charge, and

$$\frac{1}{r_0^2}\equiv\frac{1}{N}\int d^3r\,\frac{n(\mathbf{r})}{r_\perp^2} \tag{2}$$

is the average inverse-square distance of the electrons from an axis threading the ring. This result is valid for general interacting electron systems in the presence of static but otherwise arbitrary electric and magnetic fields.[2] In particular, it is valid for noninteracting electrons in a periodic potential, and we shall show that this fact leads to an unexpected—and hitherto unnoticed—constraint on the band structure of a one-dimensional crystal. Specifically, we shall prove here that the magnitude of the velocity of a Bloch electron in the nth band of a one-dimensional periodic potential is always less than or equal to the velocity of the same Bloch state in an empty lattice approximation.[3] Our inequality also implies that each energy band in a one-dimensional crystal lies below the corresponding free-electron band, when the minima of those bands are aligned.

Let $E_n(k)$ be the Bloch energy levels of an electron in a one-dimensional periodic potential of period a, where k is the crystal momentum. We shall label the energy bands according to $n=0,1,2,\ldots$, with $E_0(k)\le E_1(k)\le E_2(k)\le\cdots$, so that n bands are completely filled when the Fermi energy is in band n. The group velocity of an electron in band n is defined as

$$v_n(k)\equiv\frac{1}{\hbar}\frac{dE_n(k)}{dk}\ , \tag{3}$$

which is also equal to the expectation value of the velocity operator p/m in the Bloch state φ_{nk}. Reality of the Hamiltonian implies $E_n(k)=E_n(-k)$ and $v_n(k)=-v_n(-k)$. The existence of at most two linearly independent solutions of the Schrödinger equation at a given energy implies that the bands cannot overlap (however, they may touch, either at $k=0$ or at $k=\pi/a$, as happens in the free-electron limit). For convenience we shall define k_n to be the crystal momentum at the minimum of energy band n,

$$k_n\equiv\begin{cases}0, & n \text{ even}\\ \dfrac{\pi}{a}, & n \text{ odd.}\end{cases} \tag{4}$$

For a band structure with nonvanishing band gaps (that is, with energy bands that do not touch), the velocity clearly vanishes at k_n.

An upper bound on the magnitude of the group velocity may be obtained from the inequality $I\le I_{\max}$ as follows. Let us imagine that our one-dimensional crystal is folded into a ring of circumference L having L/a unit cells. A magnetic flux ϕ is now threaded through the center of the ring. This flux induces an equilibrium persistent current[4] $I(\phi)$, which is a periodic function of flux with period $\phi_0\equiv hc/e$. It is easy to verify that only the partially occupied band—the conduction band n—contributes to the persistent current, and that the magnitude of the *maximum* persistent current is equal to gev_F/L, where $v_F=|v_n(k_F)|$ is the magnitude of the Fermi velocity, and $g=2$ is a spin-degeneracy factor. The band index n of the partially occupied band, and the Fermi wave number k_F, may be varied to assume any desired value, by changing the number of electrons. Now, according to the inequality derived in Ref. 1,

$$\frac{gev_F}{L}\le I_{\max}\ . \tag{5}$$

Because there are n completely filled bands and one partially filled band, the total number of electrons is

$$N=gn\left[\frac{L}{a}\right]+\frac{gL}{\pi}|k_F-k_n|\ , \tag{6}$$

where we have assumed that $0\le k_F\le\pi/a$. Substituting this expression into (1), and using $L=2\pi r_0$, leads to our principal result

0163-1829/95/51(4)/2616(2)/$06.00 ©1995 The American Physical Society

$$|v_n(k)| \le \frac{\hbar}{m}\left[n\frac{\pi}{a} + \left||k| - k_n\right|\right], \tag{7}$$

valid for $(\pi/a) \le k \le (\pi/a)$.

To understand the inequality (7), we shall recall the "band structure" of free electrons, also known as the empty-lattice approximation. The energy bands in the empty lattice are given by[3]

$$E_n^0(k) \equiv \frac{\hbar^2}{2m}\left[n\frac{\pi}{a} + \left||k| - k_n\right|\right]^2, \tag{8}$$

where $-(\pi/a) \le k \le (\pi/a)$. The magnitude of the group velocity, $v_n^0(k)$, in the empty lattice is equal to

$$|v_n^0(k)| = \frac{\hbar}{m}\left[n\frac{\pi}{a} + \left||k| - k_n\right|\right]. \tag{9}$$

Therefore, our inequality (7) says that the magnitude of the velocity of a Bloch electron in one dimension is less than or equal to the magnitude of the velocity of the same state in the empty-lattice approximation,

$$|v_n(k)| \le |v_n^0(k)| . \tag{10}$$

Integrating the inequality (7) with respect to k leads to a bound on the energy bands themselves,

$$E_n(k) - E_n(k_n) \le E_n^0(k) - E_n^0(k_n) . \tag{11}$$

Therefore, each energy band must lie below the corresponding free-electron band when the minima of those bands are aligned. In particular, the actual bandwidths W_n are bounded by the free-electron bandwidths

$$W_n^0 = (2n+1)\frac{\hbar^2(\pi/a)^2}{2m} . \tag{12}$$

As a final comment, we note that it is possible to prove inequality (7) directly. We start with the well-known identity

$$\frac{1}{\hbar^2}\frac{d^2E_n}{dk^2} = \frac{1}{m} - \frac{1}{m}\sum_{n' \ne n} f_{nn'}(k) . \tag{13}$$

where

$$f_{nn'}(k) \equiv \frac{2}{m}\frac{|p_{nn'}(k)|^2}{E_{n'}(k) - E_n(k)} \tag{14}$$

are the usual oscillator strengths. Here $p_{nn'}(k) \equiv \langle \varphi_{nk}|p|\varphi_{n'k}\rangle$ are matrix elements of the momentum operator between Bloch states with the same crystal momentum. The oscillator strengths have the properties $f_{nn'}(k) \ge 0$ for $n' > n$, and $f_{nn'}(k) = -f_{n'n}(k)$. Note that

$$\int_0^{\pi/a} dk \frac{d^2E_n}{dk^2} = 0 , \tag{15}$$

so that

$$\int_0^{\pi/a} dk \sum_{n' \ne n} f_{nn'}(k) = \frac{\pi}{a} \tag{16}$$

for any band n. Also note that

$$\sum_{n'=0}^{n} \sum_{n'' \ne n'} f_{n'n''}(k) \ge 0 , \tag{17}$$

because the contribution from terms with $n'' < n$ vanishes, leaving only positive-definite oscillator strengths. This inequality implies that

$$\sum_{n' \ne n} f_{nn'}(k) \ge -\sum_{n'=0}^{n-1} \sum_{n'' \ne n'} f_{n'n''}(k) . \tag{18}$$

Next, we integrate (13) from 0 to $k \ge 0$ and use inequality (18) to obtain

$$\frac{1}{\hbar^2}\frac{dE_n}{dk} \le \frac{k}{m} + \frac{1}{m}\int_0^k dk' \sum_{n'=0}^{n-1} \sum_{n'' \ne n'} f_{n'n''}(k') . \tag{19}$$

According to (17), the integrand on the right-hand side of (19) is positive definite, so

$$\frac{1}{\hbar^2}\frac{dE_n}{dk} \le \frac{k}{m} + \frac{1}{m}\int_0^{\pi/a} dk' \sum_{n'=0}^{n-1} \sum_{n'' \ne n'} f_{n'n''}(k') , \tag{20}$$

or, upon using (16),

$$\frac{1}{\hbar^2}\frac{dE_n}{dk} \le \frac{1}{m}\left[n\frac{\pi}{a} + k\right], \tag{21}$$

valid for $0 \le k \le \pi/a$. The upper bound (21) is valid for any band n, but it is not useful for odd n, which has negative velocities for $0 \le k \le \pi/a$. However, we may also obtain a lower bound on the velocity by integrating (13) from k to π/a and using (18), which leads to

$$\frac{1}{\hbar^2}\frac{dE_n}{dk} \ge \frac{1}{m}\left[k - (n+1)\frac{\pi}{a}\right] . \tag{22}$$

For odd n and $0 \le k \le \pi/a$, this is equivalent to

$$\frac{1}{\hbar^2}\left|\frac{dE_n}{dk}\right| \le \frac{1}{m}\left[(n+1)\frac{\pi}{a} - k\right] . \tag{23}$$

The inequalities (21) and (23) together prove our upper bound (7) directly.

This work was supported by the National Science Foundation through Grant Nos. DMR-9100988 and PHY89-04035. We thank Qian Niu for a useful discussion.

*Permanent address.

[1]G. Vignale, preceding paper, Phys. Rev. B **51**, 2612 (1995).

[2]We note here that (1) is modified by current-current interactions, an order v^2/c^2 relativistic effect of the magnetic field produced at a point **r** by a moving electron at **r'**.

[3]The reduced-zone-scheme energy bands in the empty lattice approximation are obtained by folding the free-electron dispersion relation into the first Brillouin zone of the actual crystal.

[4]M. Büttiker, Y. Imry, and R. Landauer, Phys. Lett. **96A**, 365 (1983).