Newton’s law for Bloch electrons, Klein factors and deviations from canonical commutation relations

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The acceleration theorem for Bloch electrons in a homogeneous external field is usually presented using quasiclassical arguments. In quantum mechanical versions the Heisenberg equations of motion for an operator \( \hat{\mathbf{k}}(t) \) are presented mostly without properly defining this operator. This leads to the surprising fact that the generally accepted version of the theorem is incorrect for the most natural definition of \( \hat{\mathbf{k}} \). This operator is shown not to obey canonical commutation relations with the position operator. A similar result is shown for the phase operators defined via the Klein factors which take care of the change of particle number in the bosonization of the field operator in the description of interacting fermions in one dimension. The phase operators are also shown not to obey canonical commutation relations with the corresponding particle number operators. Implications of this fact are discussed for Tomonaga-Luttinger type models.

I. INTRODUCTION

The problem of the electronic motion in a crystal subject to a homogeneous electric field is treated in virtually all textbooks on solid state physics. Using semiclassical arguments one arrives at the \( \mathbf{k} \)-space form of Newton’s law for Bloch waves

\[
\frac{\hbar}{m_e} \frac{d\mathbf{k}}{dt} = \mathbf{F}
\]

(1)

where \( \mathbf{F} = e\mathbf{E} \), with \( \mathbf{E} \) the electric field, is a spatially uniform force \( \mathbf{F} \). In more advanced texts discussions are presented that this law also holds rigorously as a quantum mechanical law, when \( \hat{\mathbf{k}}(t) \) is interpreted as the expectation value of an operator \( \hat{\mathbf{k}} = e^{i\mathbf{H}t} \hat{\mathbf{k}} e^{-i\mathbf{H}t} \) for an arbitrary wave packet \( |\psi⟩ \). In this paper we will point out various subtleties in the definition of the operator \( \hat{\mathbf{k}} \), which surprisingly are not sufficiently discussed in the literature.

It is well-known that there are certain mathematical problems with the fact that the perturbation \( -\mathbf{F} \cdot \hat{\mathbf{x}} \) is an unbounded operator. This has led to a long discussion about the existence of localized eigenstates, so-called “Wannier-Stark-ladders”. It has been shown that the problem is very different if one restricts the Hilbert space to a finite number of Bloch bands or works in the full Hilbert space. As the important aspects of the problem show up already in one-dimensional systems we restrict our discussion to this case. A little more mathematical sophistication than usual in solid state physics is required to appreciate the importance of a proper definition of the operator \( \hat{\mathbf{k}} \). Take for example the single band case discussed in section III and let \( |E_0⟩ \) be a localized Wannier-Stark eigenstate of the Hamiltonian. Then obviously \( \langle E_0 | \hat{\mathbf{k}}(t) | E_0 ⟩ = \langle E_0 | \hat{\mathbf{k}} | E_0 ⟩ \), i.e. the expectation value is time-independent in contradiction to Eq. (1). The solution to this problem has some similarity to the subtleties of the canonical commutation relations for a particle on a ring. But there the wave function itself is defined on a compact space, while this is not the case for the Bloch electron in a homogeneous field where the periodicity enters via the \( \mathbf{k} \)-space classification of the eigenstates in a periodic potential. A similar problem occurs in a proper definition of the so-called “Klein-factors” \( U \), which in the method of “bosonization” take proper care of the change of the number of particles, when the electronic field operator is expressed in terms of boson operators. The \( U \) are unitary operators and as such can be expressed as \( U = e^{iM} \), where \( M \) is a self-adjoint operator. We will show in this paper, that, given \( U \) the operator \( M \) remains undetermined to a larger extent than one could naively expect. But whatever choice one takes, this operator \( M \) can be shown not to obey the commutation relation with the particle number which is widely assumed.

In section II we discuss the problem of an electron in a periodic potential and a homogeneous external field. First introducing the translation operator \( \hat{T}_a \) by a lattice spacing, different definitions of the operator \( \hat{k} \) are given, which all lead to \( \hat{T}_a = e^{-i\mathbf{k}a} \), but different forms of Newton’s law and commutation relations with the position operator. The most obvious choice for \( \hat{k} \) does not lead to Newton’s law in the form of Eq. (1) and allows to resolve the contradiction for the case of Wannier-Stark states mentioned above. In section III we discuss the problem, when the Hilbert space is restricted to a finite number of bands. The results of sections II and III can directly be used for the discussion of the Klein operators in section IV. We finally discuss the implications in the rather different situations where the same mathematical problem shows up in section V.

II. A BLOCH ELECTRON IN A HOMOGENEOUS FIELD

In this section we discuss the motion of an electron in a periodic potential \( V(x) = V(x + a) \), where \( a \) is the lattice constant, subject to an additional homogeneous external
\[ \hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) - F\hat{x}. \]  

In the attempt to derive the \( k \)-space form of Newton's law it is useful to introduce the translation operator \( \tilde{T} \), which (actively) shifts the state by one lattice spacing to the right \( \langle x|\tilde{T}_a|\psi\rangle = \langle x - a|\psi\rangle \). The commutator of \( \tilde{T}_a \) with the Hamiltonian is given by

\[ [\tilde{T}_a, \hat{H}] = [\tilde{T}_a, -F\hat{x}] = aF\tilde{T}_a \]  

Therefore the Heisenberg equation of motion \( i\hbar \tilde{T}_a(t) = [\tilde{T}_a, \hat{H}](t) \) has the solution

\[ \tilde{T}_a(t) = \tilde{T}_a e^{-iaFt/\hbar}. \]  

As it is well known from elementary quantum mechanics books the most obvious way to present the translation operator is \( \tilde{T}_a = e^{-iap/\hbar} \), where \( \hat{p} \) is the momentum operator. This is not the appropriate choice in the following. We nevertheless show which contradictions one seems to find but calculate anyway and first discuss the case \( \hat{p}/\hbar \equiv \hat{\mathbf{p}} \) reads

\[ e^{-iap(t)/\hbar} = e^{-ia(\hat{p} + F\hat{\mathbf{t}})/\hbar}. \]  

Obviously it is not allowed to infer \( \hat{\mathbf{p}}(t) = \hat{p} + F\hat{\mathbf{t}}/\hbar \) from this equation, as it contradicts for all \( V \neq 0 \) the Heisenberg equation of motion

\[ \dot{\hat{p}}(t) = -\frac{\partial V}{\partial x}(\hat{x}(t)) + F\hat{\mathbf{1}}. \]  

We postpone the discussion of what goes wrong with this argument and first discuss the case \( V = 0 \), i.e. a system without the periodic potential (“empty lattice”), where no contradiction arises. The spectral decomposition of \( \hat{\mathbf{p}} \equiv \hat{\mathbf{p}}/\hbar \) reads

\[ \hat{\mathbf{p}} = \int_{-\infty}^{\infty} |k\rangle \langle k| \text{dk}, \]  

where the \( |k\rangle \) are plane wave states \( \langle x|k\rangle = e^{ikx}/\sqrt{2\pi} \), which are normalized as \( \langle k|k'\rangle = \delta(k-k') \). In order to find \( \hat{\mathbf{p}}(t) \) we do not proceed the simple way using Eq. (6) but calculate \( \langle k(-t)| \langle k(-t)| \rangle \) needed later. The operator \( \hat{P}_{0,k} \equiv |k\rangle \langle k| \) commutes with the kinetic energy and its commutator with \( \hat{x} \) follows using \( \langle k|\hat{x}|\psi\rangle = i\frac{\partial}{\partial k}\langle k|\psi\rangle \) as \( \langle \hat{P}_{0,k}, \hat{x}\rangle = i\frac{\partial}{\partial k}\hat{P}_{0,k} \). For \( V = 0 \) this leads to the equation of motion

\[ i\hbar \frac{\partial}{\partial t} \hat{P}_{0,k}(t) = -iF\frac{\partial}{\partial k} \hat{P}_{0,k}(t) \]  

with the solution \( \hat{P}_{0,k}(t) = \hat{P}_{0,k-Ft/\hbar}(0) \), i.e. \( |k(-t)| \langle k(-t)| \rangle = |k - Ft/\hbar\rangle \langle k - Ft/\hbar| \). Using Eq. (7) this yields the result expected from Eq. (6)

\[ \hat{k}(t) = \int_{-\infty}^{\infty} |k - Ft/\hbar\rangle \langle k - Ft/\hbar| \text{dk} = \hat{\mathbf{k}} + F\hat{\mathbf{t}}. \]

This shows explicitly that for \( V = 0 \) just comparing the exponents in Eq. (5) provides the correct answer.

We now address the question of how much an operator \( \hat{k} \) can differ from \( \hat{\mathbf{k}} \) defined in Eq. (7) and nevertheless yield \( \tilde{T}_a = e^{-ika} \). To answer this we consider an arbitrary projection operator \( \hat{P} = \hat{P}^2 \). Simply expanding the exponential function leads to the identity

\[ e^{ia\hat{P}} = \hat{1} + (e^{ia} - 1) \hat{P}. \]

For \( \alpha = 2\pi n \), with \( n \) integer this simplifies to

\[ e^{2\pi i\alpha \hat{P}} = \hat{1}. \]

If two operators \( \hat{A} \) and \( \hat{B} \) fulfill \( e^{iA} = e^{iB} \) multiplication with \( e^{2\pi i\alpha \hat{P}} = \hat{1} \) yields \( e^{i\hat{A}} = e^{i\hat{B} + 2\pi i\alpha \hat{P}} \). If \( \hat{P} \) commutes with \( \hat{B} \), one obtains \( e^{i\hat{A}} = e^{i(\hat{B} + 2\pi i\alpha \hat{P})} \), i.e. \( \hat{A} \) and \( \hat{B} \) can differ by \( 2\pi i\alpha \hat{P} \) and still fulfill \( e^{i\hat{A}} = e^{i\hat{B}} \). If \( \hat{B} \) is a self-adjoint operator with the spectral decomposition

\[ \hat{B} = \sum_b |b\rangle b\langle b| \]

every restricted sum (integral) \( \hat{P} = \sum_b |b\rangle b\langle b| \) is a projector which commutes with \( \hat{B} \). This simple observation is essential for the problem addressed in this paper.

As a first application we write \( k \) in the integrand in Eq. (7) in the form \( k = \hat{k} + \frac{2\pi n}{a} \), with \( n \) integer and \( \hat{k} \in [-\pi/a, \pi/a] \). Then we can rewrite this equation in the form

\[ \hat{k} = \sum_{n=-\infty}^{\infty} \int_{-\pi/a}^{\pi/a} |k + \frac{2\pi n}{a}\rangle \langle k + \frac{2\pi n}{a}| \text{dk} \]

\[ = \sum_{n=-\infty}^{\infty} \int_{-\pi/a}^{\pi/a} |k + \frac{2\pi n}{a}\rangle \langle k + \frac{2\pi n}{a}| \text{dk} \]

\[ + \sum_{n=-\infty}^{\infty} \frac{2\pi}{a} \int_{-\pi/a}^{\pi/a} \langle k + \frac{2\pi n}{a}| \langle k + \frac{2\pi n}{a}| \text{dk} \]

\[ = \hat{k}_b + \sum_{n=-\infty}^{\infty} \frac{2\pi}{a} \hat{\mathbf{p}}(n), \]  

where now \( \hat{k}_b \) is a bounded operator, and the projection operators \( \hat{P}(n) \) commute with \( \hat{k}_b \), i.e. we also have \( \tilde{T}_a = e^{-iak_b} \). In the position representation \( \hat{k}_b \) is a nonlocal operator.
\[\langle x | \hat{K}^{(a)}_b | \psi \rangle = \int_{-\infty}^{\infty} \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} e^{i\frac{2\pi}{a}n(x-x')} \times \left( \int_{-\pi/a}^{\pi/a} k e^{ik(x-x')} dk \right) \psi(x') dx'\]

\[= \frac{1}{t} \int_{-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \delta(x-x' - ma) \times \left[ \cos \left( \frac{(x-x')\pi/a}{(x-x')} \right) - a \sin \left( \frac{(x-x')\pi/a}{\pi(x-x')^2} \right) \right] \psi(x') dx' \]

\[= \sum_{m=1}^{\infty} \left( \frac{1}{t} \right)^m \left[ \psi(x-ma) - \psi(x+ma) \right], \quad (14)\]

where we have used Eq. (A1). In the following we suppress the \(a\)-dependence of the operator \(\hat{K}^{(a)}_b\). In order to discuss \(\hat{K}_b(t)\) it is convenient to introduce the operators

\[\hat{P}_k \equiv \sum_{n=-\infty}^{\infty} |k + \frac{2\pi a}{n}| \langle k + \frac{2\pi a}{n} | = \hat{P}_k + \frac{2\pi}{a} m, \quad (15)\]

where we have indicated that they are periodic in the reciprocal lattice \((m \in \mathbb{Z})\) and we have

\[\hat{k}_b = \int_{-\pi/a}^{\pi/a} \hat{P}_k dk. \quad (16)\]

If for \(V = 0\) we again use \(|k(-t)| (k(-t)) = |k - Ft/h| (k - Ft/h)| we obtain \(\hat{P}_k(t) = \hat{P}_k \cdot F \cdot \hat{P}_k\). Because of the periodicity \(\hat{P}_k = \hat{P}_k + \frac{2\pi}{a} m\) we have \(\hat{P}_k(t) = \hat{P}_k(t+nT)\) where \(T = \frac{2\pi}{a} F\), and we can restrict the following discussion to times \(t \in [0, T]\)

\[\hat{k}_b(t) = \int_{-\pi/a}^{\pi/a} \hat{P}_{k-F\cdot t/h} dk \]

\[= \int_{-\pi/a}^{\pi/a} \hat{P}_{k-F\cdot t/h+2\pi/a} dk + \int_{-\pi/a}^{\pi/a} \hat{P}_{k-F\cdot t/h} dk, \quad (17)\]

where we have used Eq. (15). Now we can substitute \(k' = k - Ft/h + 2\pi/a\) in the first term and \(k' = k - Ft/h\) in the second. This yields

\[\hat{k}_b(t) = \int_{-\pi/a}^{\pi/a} (k' - Ft/h - 2\pi/a) \hat{P}_{k'} dk'\]

\[+ \int_{-\pi/a}^{\pi/a} (k' + Ft/h) \hat{P}_{k'} dk' \quad (18)\]

Apart from the term proportional to \(2\pi/a\) we can recombine the integrals and obtain using \(\int_{-\pi/a}^{\pi/a} \hat{P}_k dk = 1\)

\[\hat{k}_b(t) = \hat{k}_b + Ft/h \hat{1} - \frac{2\pi}{a} \int_{-\pi/a}^{\pi/a} \hat{P}_k dk, \quad (19)\]

Comparing with Eq. (9) we see that the expressions of \(\hat{k}(t)\) and \(\hat{k}_b(t)\) in terms of \(\hat{k}\) and \(\hat{k}_b\) differ by the last term on the rhs of Eq. (19). We will discuss its implications after we show that in fact Eq. (19) also holds in the presence of the periodic potential. We denote the eigenstates of \(\hat{H}_0 = \hat{p}^2/2m + V(\hat{x})\) by \(|k, \alpha\rangle\)

\[\hat{H}_0 |k, \alpha\rangle = \epsilon_{k,\alpha} |k, \alpha\rangle, \quad (20)\]

where \(k\) is the wave vector in the first Brillouin zone and \(\alpha\) is the band index. When the states are normalized as \(|\langle k, \alpha |k', \alpha'\rangle = \delta_{\alpha,\alpha'} \delta(k-k')\) they provide a decomposition of the unit operator

\[\sum_{\alpha} \int_{-\pi/a}^{\pi/a} |k, \alpha\rangle \langle k, \alpha| dk = \hat{1}. \quad (21)\]

In the appendix we present the simple proof that the \(\hat{P}_k\)

can also be expressed in terms of the Bloch states

\[\hat{P}_k = \sum_{n=-\infty}^{\infty} |k + \frac{2\pi a}{n}| \langle k + \frac{2\pi a}{n} | = \sum_{\alpha} |k, \alpha\rangle \langle k, \alpha| \quad (22)\]

The Heisenberg equation of motion for \(\hat{P}_k(t)\) reads

\[i\hbar \frac{d}{dt} \hat{P}_k(t) = -\frac{\hbar}{\partial t} \hat{P}_k(t) - F \left[ \hat{P}_k(t), \hat{x} \right] (t) \quad (23)\]

If one uses the expression for \(\hat{P}_k\) in terms of the Bloch states the first term on the rhs is seen to vanish, while the expression using the plane waves shows that \[\hat{P}_k, \hat{x}\] and Eq. (23) simplifies to \(\hbar \frac{d}{dt} \hat{P}_k(t) + F \frac{\partial}{\partial k} P_k(t) = 0\). This leads to the solution

\[\hat{P}_k(t) = \hat{P}_k(-Ft/h)(0), \quad (24)\]

which expresses the well known fact that a state with a single sharp value of \(k\) remains a state with a single sharp value of \(k\), independent of any interband transitions. The further steps for the calculation of \(\hat{k}_b(t)\) are identical to Eqs. (16-19). Therefore Newton’s law for Bloch electrons in a homogeneous field has the solution \(\hat{k}_b(t) = \hat{k}_b(t + nT)\) and for \(t \in [0, T]\)

\[\hat{k}_b(t) = \hat{k}_b + Ft/h \hat{1} - \frac{2\pi}{a} \sum_{\alpha} \int_{-\pi/a}^{\pi/a} |k, \alpha\rangle \langle k, \alpha| dk \quad (25)\]

This one of the central results of the present paper. The last term on the rhs of Eq. (25) is missing in all presentations of the “acceleration law” known to me. Its appearance can be traced to the fact that the operators \(\hat{P}_k\) are periodic in the reciprocal lattice. A similar term has been discussed previously in connection with a free particle on a ring. If one calculates expectation values with a general wave packet \(|\psi\rangle = \sum_{\beta} \int_{-\pi/a}^{\pi/a} a_\beta(k) |k, \beta\rangle dk\) the expectation
value of \( \langle \hat{k}_b(t) \rangle = \langle \hat{k}_b(t + nT) \rangle \) for \( t \in [0, T] \) is given by

\[
\langle \hat{k}_b(t) \rangle = \langle \hat{k}_b \rangle + Ft/\hbar - \frac{2\pi}{a} \sum_\beta \int_{\pi/a-Ft/\hbar}^{\pi/a} |a_\beta(k)|^2 dk,
\]

with \( \langle \hat{k}_b \rangle = \sum_\beta \int_{-\pi/a}^{\pi/a} |a_\beta(k)|^2 dk \). For a wave packet initially strongly peaked around a wave number \( k_0 \), the expectation value \( \langle \hat{k}_b(t) \rangle \) closely follows the saw-tooth curve shown in Fig. 1 except at the “times of the Bragg-reflections”. This implies that Eq. (1) holds to a good approximation except during these reflections, when \( k \) is identified with \( \langle \hat{k}_b(t) \rangle \). For an arbitrary wave packet this is not the case due to the additional term from differentiating the last term on the rhs of Eq. (26). This can be clearly seen in Fig. 1.

The additional term on the rhs of Eq. (25) allows to resolve the contradictions mentioned in the introduction. This will be discussed in the next section. It also leads to an additional term in the commutator \([\hat{x}, \hat{k}_b]\) compared to \([\hat{x}, \hat{k}] = i\). If we compare the Heisenberg equation of motion \( i\hat{k}_b(t) = [\hat{k}_b, H](t) = -F \left[ \hat{k}_b, \hat{x} \right] \) for \( t = 0 \) with Eq. (25) differentiated with respect to time we readily obtain

\[
\left[ \hat{x}, \hat{k}_b \right] = i \left( 1 - \frac{2\pi}{a} \sum_\alpha \left( \frac{\pi}{a}, \alpha \right) \left( \frac{\pi}{a}, \alpha \right) \right),
\]

i.e. \( \hat{x} \) and \( \hat{k}_b \) do not obey canonical commutation relations. If one goes over from \( \hat{k}_b \) to \( \hat{k}_b \) by adding \( 2\pi n \hbar \hat{P}/a \), where \( \hat{P} \) is a projection operator commuting with \( \hat{k}_b \), additional terms appear on the rhs of Eq. (27). A detailed discussion of the additional term is given in the next section, where we also present an alternative derivation of the result.

### III. Description in a Restricted Hilbert Space

The description of a Bloch electron in the external field simplifies considerably when the dynamics of an initial state in the form of a wave packet in a single band is considered and interband transitions are neglected. In this approximation the electron undergoes “Bloch oscillations” i.e. \( \langle \hat{x}(t) \rangle \) is periodic in time. A first step beyond this simple approximation is a two-band model which provides a good description for the dynamics of electrons in high quality semiconductor superlattices, with a pair of isolated minibands. More generally the \( N \)-band approximation amounts to the replacement

\[
\hat{H}_0 \rightarrow \sum_{i=1}^{N} \int_{-\pi/a}^{\pi/a} [k, \alpha_i] \zeta_{k, \alpha_i} \delta_{k, \alpha_i} dk,
\]

and the restriction of the operator \( \hat{x} \) to the Hilbert space spanned by the \( N \) bands. In the following it is useful also to work with Wannier states

\[
|m, \alpha\rangle = \sqrt{\frac{a}{2\pi}} \int_{-\pi/a}^{\pi/a} e^{-ikm} |k, \alpha\rangle dk,
\]

which are localized around the \( m \)-th lattice site, i.e. \( \langle x|m, \alpha\rangle = a_m(x - ma) \). They are orthonormal \( \langle m, \alpha|n, \beta\rangle = \delta_{m,n} \delta_{\alpha,\beta} \) and therefore can also be used for a decomposition of the unit operator in the restricted \( N \)-band Hilbert space. Elementary calculation yields for the Wannier matrix elements of the position operator

\[
\langle m, \alpha|x|n, \beta\rangle = ma \delta_{mn} \delta_{\alpha,\beta} + \Omega_{\alpha\beta}^{m-n}
\]

\[
\Omega_{\alpha\beta}^{m-n} = \int_{-\infty}^{\infty} dx \ a_n^*(x)a_{m+n} \left( x + (m-n)a \right)
\]

with \( \Omega_{\alpha\beta}^{m-n} \) which implies for the Bloch state matrix elements using (A.1)

\[
\langle k, \alpha|x|k', \beta\rangle = \delta_{\alpha,\beta} \delta(2\pi/a)(k - k') + \delta(2\pi/a)(k - k') \Omega_{\alpha\beta}(k),
\]

with \( \Omega_{\alpha\beta}(k) = \sum_{l} e^{-ikl} \Omega_{\alpha\beta}^{l} \) which defines the Bloch state matrix elements in (A.1). In the following we suppress the index “2\( \pi/a \)” of the delta functions as wave numbers are always restricted to the first Brillouin zone.

The translation operator \( \hat{T}_a \) when acting on a Wannier state changes \( m \) by one, i.e. \( \hat{T}_a|m, \alpha\rangle = |m+1, \alpha\rangle \). Therefore the restriction \( T_a(N) \) on the \( N \)-band space has
the simple form
\[
\hat{T}_a^{(N)} = \sum_{i=1}^{N} \sum_{m=-\infty}^{\infty} |m + 1, \alpha_i \rangle \langle m, \alpha_i |
\] (32)

From the inverse relation of Eq. (29)
\[
|k, \alpha \rangle = \sqrt{\frac{a}{2\pi}} \sum_{m=-\infty}^{\infty} e^{ikam} |m, \alpha \rangle
\] (33)

it follows that \(\hat{T}_a^{(N)}|k, \alpha \rangle = e^{-ika}|k, \alpha \rangle\) and therefore \(\hat{T}_a^{(N)}\) \(k, \alpha \) can be written as \(\hat{T}_a^{(N)} = \exp (-iak_b)\) with
\[
\hat{k}_b^{(N)} = \sum_{i=1}^{N} \int_{\pi/a}^{\pi/a} |k, \alpha_i \rangle \langle k, \alpha_i |dk \equiv \int_{\pi/a}^{\pi/a} \hat{P}_k^{(N)} dk .
\] (34)

The only difference to section II is therefore the restricted sum over bands. In the equation of motion for \(\hat{P}^{(N)}(t)\) one again has to determine the commutator with the position operator. As now there is no equivalent to Eq. (22) the argument presented in appendix A cannot be used. Using Eq. (31) it is straightforward to show that
\[
\left[ \hat{x}^{(N)}, \hat{P}_k^{(N)} \right] = i \frac{\partial}{\partial k} \hat{P}_k^{(N)}
\] (35)

by calculating matrix elements in Bloch states of both sides of this equation. Then all further arguments of section II can be used and one obtains \(\hat{k}_b^{(N)}(t) = \hat{k}_b^{(N)}(t + \alpha T)\) and for \(t \in [0, T]\)
\[
\hat{k}_b^{(N)}(t) = \hat{k}_b^{(N)}(t) + \langle N \rangle Ft/\hbar
\] (36)
\[
-\frac{2\pi}{a} \sum_{i=1}^{N} \int_{\pi/a}^{\pi/a} |k, \alpha_i \rangle \langle k, \alpha_i |dk .
\]

Again the only difference to section II is the restricted sum over bands. The main new physics is that for the restricted \(N\)-band Hilbert space localized eigenstates \(E_n^\mu = \langle \hat{T}_a^{(N)} \rangle^n |E_0^\mu \rangle \) of \(\hat{H}^{(N)} - \hat{F}_{\alpha}^{(N)}\), with \(n \in \mathbb{Z}\) and \(\mu = 1, \ldots, N\) are known to exist. The corresponding energies \(E_n^\mu\) form \(N\) “Wannier-Stark” ladders
\[
E_n^\mu = E_0^\mu - n\alpha F.
\] (37)

This property is easily shown using
\[
\left( \hat{T}_a^{(N)} \right)^{-1} \hat{H}^{(N)} \hat{T}_a^{(N)} - H^{(N)} - F_{\alpha} 1 .
\]

Now we can resolve the contradiction of \(\langle E_n^\mu | \hat{k}_b^{(N)}(t) | E_n^\mu \rangle = \langle E_n^\mu | \hat{k}_b^{(N)} | E_n^\mu \rangle\) with Eq. (1) mentioned in the introduction. The last term on the rhs of Eq. (36) avoids to allow the inconsistency. If one takes the expectation value of Eq. (36) with the normalized eigenstate \(E_n^\mu\) and differentiates with respect to time one finds that \(d \langle E_n^\mu | \hat{k}_b^{(N)}(t) | E_n^\mu \rangle /dt = 0\) is fulfilled if
\[
\sum_{i=1}^{N} |\langle k, \alpha_i | E_n^\mu \rangle|^2 = \frac{a}{2\pi}
\] (38)
holds. In order to see that this in fact is true one has to examine the time-independent Schrödinger equation \(\hat{H}^{(N)} |E_n^\mu \rangle = E_n^\mu |E_n^\mu \rangle\). Using Eq. (31) it reads in Bloch representation
\[
\frac{i}{\hbar} \frac{\partial}{\partial k} (k, \alpha_i | E_n^\mu \rangle = \left( - \frac{E_n^\mu - \varepsilon_{k, \alpha_i}}{F} \right) (k, \alpha_i | E_n^\mu \rangle
\]
\[
- \sum_{j=1}^{N} \Omega_{\alpha_i, \alpha_j} (k, \alpha_j | E_n^\mu \rangle . (39)
\]

With \(k \to t\) this looks like a “time” dependent Schrödinger equation with a “time” dependent Hermitian \(N \times N\) Hamiltonian matrix. The “conservation of probability” immediately shows that the lhs of Eq. (38) is \(k\)-independent. Integration over the first Brillouin zone allows to use the completeness relation. Because of \(\langle E_n^\mu | E_n^\mu \rangle = 1\) this immediately proves Eq. (38). In the simplest case \(N = 1\) Eq. (39) is a single first order linear differential equation and can be trivially integrated and allows an analytical discussion of the eigenstates \(|E_n \rangle\) in real space.

It is instructive to write the operator \(\hat{k}_b\) in Eq. (34) also in the Wannier representation. If one performs the simple integration as in Eq. (14) in \(\langle m, \alpha | \hat{k}_b^{(N)} | n, \beta \rangle = \delta_{\alpha, \beta} \langle m, \alpha | \hat{k}_b^{(N)} | n, \alpha \rangle\) one obtains
\[
\hat{k}_b^{(N)} | n, \alpha \rangle = \sum_{m(\neq n)} (-1)^{m-n} \frac{(-1)^{m-n}}{(m-n)a} |m, \alpha \rangle . (40)
\]

As the \(\langle m, \alpha | \hat{k}_b^{(N)} | n, \beta \rangle\) decay as \(1/|m-n|\) for \(|m-n| \to \infty\), the states \(\hat{k}_b | n, \alpha \rangle\) lie in the Hilbert space \(\mathcal{H}_N\) spanned by the Wannier states of the \(N\) bands. If one would take Eq. (40) as the definition of the operator \(\hat{k}_b\) it is straightforward to show using Eqs. (33) and (40) that
\[
\hat{k}_b^{(N)} | k, \alpha \rangle = \left( 2 \sum_{l=1}^{\infty} \frac{(-1)^{l+1}}{la} \sin kla \right) |k, \alpha \rangle
\] (41)
\[
\equiv f_{st}(k) |k, \alpha \rangle,
\]
where \(f_{st}(k)\) is the periodic saw tooth curve which is given by \(f_{st}(k) = k\) in the first Brillouin zone. The use of Eq. (40) also allows an alternative derivation of the restricted Hilbert space commutation relation corresponding to Eq. (27). For that purpose we decompose the position operator using Eq. (30) as \(\hat{x}^{(N)} \equiv \hat{x}_d^{(N)} + \hat{x}_\Omega^{(N)}\) with
\[
\hat{x}_d^{(N)} = \sum_{i=1}^{N} \sum_{m} |m, \alpha_i \rangle a m \langle m, \alpha_i | . (42)
\]

This part of the position operator, which is diagonal in the Wannier representation, leads to the nonvanishing commutator with \(\hat{k}_b^{(N)}\). As \(\hat{x}_d^{(N)} | m, \alpha_i \rangle = a m |m, \alpha_i \rangle\) the
states $\hat{z}_d^{(N)}|m,\alpha_i\rangle$ as well as the states $\hat{k}_b^{(N)} \hat{z}_d^{(N)}|m,\alpha_i\rangle$ are normalizable and therefore elements of $\mathcal{H}_N$. If on the other hand $\hat{k}_b^{(N)}$ is applied first, one obtains

$$\hat{z}_d^{(N)} \hat{k}_b^{(N)}|n,\alpha_i\rangle = \sum_{m(\neq n)} \left(\frac{-1}{m-n}\right)|m,\alpha_i\rangle. \quad (43)$$

These states are not normalizable and therefore (like the Bloch states) strictly speaking not elements of the Hilbert space $\mathcal{H}_N$. If one nevertheless formally calculates the commutator of $\hat{z}_d^{(N)}$ and $\hat{k}_b^{(N)}$ it is given by

$$\Big[\hat{z}_d^{(N)}, \hat{k}_b^{(N)}\Big]|n,\alpha_i\rangle = -i \sum_{m(\neq n)} (-1)^{n-m} |m,\alpha_i\rangle = i \left(n,\alpha_i\right) - (-1)^n \sum_m (-1)^m |m,\alpha_i\rangle. \quad (44)$$

The first form shows e.g. that the diagonal elements in the Wannier representation of the commutator vanish, i.e. it cannot be proportional to the unit operator. If Eq. (44) is multiplied by $|n,\alpha_i\rangle$ from the right and summations over $n$ and $\alpha$ are carried out, the expression for the commutator reads

$$\Big[\hat{z}_d^{(N)}, \hat{k}_b^{(N)}\Big] = i \left(\hat{1}_N - \frac{2\pi}{\alpha} \sum_{i=1}^{N} \left| k = \frac{\pi}{\alpha}, \alpha_i \right\rangle \left\langle k = \frac{\pi}{\alpha}, \alpha_i \right|\right), \quad (45)$$

which is the analog of Eq. (27) for the case of the restricted Hilbert space. As in section II it could have been derived also by using the derivative of Eq. (36) at $t = 0$ and using Eq. (31) to see that $\hat{z}_d^{(N)}$ commutes with $\hat{k}_b^{(N)}$. In the next section we discuss how the above commutation relation occurs in a completely different context. There the analog of the Wannier states is the starting point of the description.

**IV. BOSONIZATION AND KLEIN OPERATORS**

In this section we first present a very short introduction to the ideas behind bosonization, which is a very successful technique for treating interacting fermions in one dimension. Consider a system of fermions with one-particle basis states $|l\rangle$ and the corresponding annihilation operators $c_l$, where $l \in \mathbb{Z}$ is a quantum number running from $-M_0$ to $\infty$. For spinless particles in a 1D box with hard walls $M_0 = \frac{1}{2}$. In the treatment for interacting fermions Luttinger introduced the purely technical device to add “unphysical” one particle states with negative $l$ and considered the limit $M_0 \to \infty$. In order to avoid mathematical subtleties it is more transparent to introduce the concept of bosonization for finite $\hat{M}_0$ and to perform the limit $\hat{M}_0 \to \infty$ later. The state where the lowest one particle states from $-\hat{M}_0$ to $N$ are occupied is denoted by $|\{0\},N\rangle$, where the symbol $\{0\}$ is introduced, because instead of using fermionic occupation numbers it is possible to work with $N + \hat{M}_0 + 1$-particle basis states

$$|\{m\},N\rangle = \prod_{l>0} \left(\frac{b_l^\dagger}{{\sqrt{m_l}}}\right) |\{0\},N\rangle, \quad (46)$$

where the operators $b_l^\dagger$ with $l \geq 1$ are defined as

$$b_l^\dagger = \frac{1}{\sqrt{l}} \sum_{n=-\hat{M}_0}^\infty c_{n+l}^\dagger c_n. \quad (47)$$

In the limit $\hat{M}_0 \to \infty$ these operators obey Bose commutation relations $[b_l^\dagger, b_m^\dagger] = 0$ and

$$[b_l, b_m^\dagger] = \delta_{lm} 1, \quad (48)$$

while for finite $\hat{M}_0$ Eqs. (46) and (48) only hold for low lying excited states. If the fermions have spin, all operators have additional spin labels. For the point about “Klein factors” we want to make, it is sufficient to work with the auxiliary field operator $\hat{\psi}(v)$ which in the limit $\hat{M}_0 \to \infty$ is defined as

$$\hat{\psi}(v) = \sum_{l=-\infty}^\infty e^{ivc_l}. \quad (49)$$

Its commutation relations with the Bose operators are

$$[b_m, \hat{\psi}(v)] = -\frac{1}{\sqrt{m}} e^{-imv} \hat{\psi}(v),$$

$$[b_m^\dagger, \hat{\psi}(v)] = -\frac{1}{\sqrt{m}} e^{imv} \hat{\psi}(v). \quad (50)$$

The essential observation for the “bosonization” of $\hat{\psi}$ is the fact that exponentials of Bose operators obey analogous commutation relations

$$[b_m, e^{-\sum_{n=1}^{\infty} \frac{imv}{\sqrt{n}}} b_n^\dagger] = -\frac{1}{\sqrt{m}} e^{-imv} e^{-\sum_{n=1}^{\infty} \frac{imv}{\sqrt{n}}} b_n^\dagger b_n \quad (51)$$

$$[b_m^\dagger, e^{\sum_{n=1}^{\infty} \frac{imv}{\sqrt{n}}} b_n] = -\frac{1}{\sqrt{m}} e^{-imv} e^{\sum_{n=1}^{\infty} \frac{imv}{\sqrt{n}}} b_n. \quad (52)$$

Eqs. (50) and (51) imply that $\hat{O}(v)$ commutes with the $b_n$ and $b_n^\dagger$. As the exponentials in Eq. (52) conserve the particle number, the Klein operator $\hat{O}(v)$ has to lower the particle number by one as the field operator on the lhs of
the equation. In the following an explicit construction of $\hat{O}(v)$ is presented, which considerably simplifies earlier approaches. The first step is to show that the state $\hat{O}(v)|\{0\}, N\rangle$ has no overlap to excited states. Using

\begin{align}
\langle m_l, N - 1|\hat{O}(v)|\{0\}, N\rangle = \\
\prod_l \frac{1}{\sqrt{m_l!}} \langle \{0\}, N - 1| (b_l)^{m_l} \hat{O}(v)|\{0\}, N\rangle
\end{align}

and the fact that $\hat{O}(v)$ commutes with the $b_l$, the rhs of Eq. (53) is seen to vanish unless all $m_l$ are zero, as $b_l|\{0\}, N\rangle = 0$. This implies

$$
\hat{O}(v)|\{0\}, N\rangle = c_N(v)|\{0\}, N - 1\rangle,
$$

(54)

where $c_N(v)$ is a c-number. In order to determine $c_N(v)$ we calculate $\langle \{0\}, N - 1|\hat{v}(v)|\{0\}, N\rangle$ using Eq. (49) and compare with the result when Eqs. (52) and (54) are used. This yields $c_N(v) = e^{iNv}$. If Eq. (54) is multiplied by $\prod_l (b_l)^{m_l}/\sqrt{m_l!}$ from the left, the fact that $\hat{O}(v)$ commutes with the $b_l$ completely determines $\hat{O}(v)$

$$
\hat{O}(v)|\{m_l\}, N\rangle = e^{iNv}|\{m_l\}, N - 1\rangle.
$$

(55)

Using the completeness of the states $|\{m_l\}, N\rangle$ one can write Eq. (55) in the form

$$
\hat{O}(v) = \hat{U} e^{i\hat{N}v}
$$

(56)

where $\hat{N}$ is the particle number operator relative to the Dirac see

$$
\hat{N} = \sum_{\{m_l\}} \sum_N |\{m_l\}, N\rangle N \langle \{m_l\}, N|
$$

(57)

and the particle number changing part $\hat{U}$ which is independent of $v$ is given by

$$
\hat{U} = \sum_{\{m_l\}} \langle \{m_l\}, N - 1|\langle \{m_l\}, N|
$$

(58)

If one identifies the particle number $N$ with the site index and the $\{m_l\}$ with the $\alpha_i$ in Eq. (32), the operator $\hat{U}$ has the form of a translation operator $T_{-\alpha}$, which shifts the system to the left by one lattice site. Therefore the eigenstates of $\hat{U}$ are the corresponding “Bloch states”

$$
|m_l\rangle \equiv \frac{1}{\sqrt{2\pi}} \sum_{N=-\infty}^{\infty} e^{i\alpha N} |\{m_l\}, N\rangle.
$$

(59)

Now one can again write $\hat{U} = e^{i\hat{k}}$ with

$$
\hat{k} \equiv \sum_{\{m_l\}} \int^\pi_{-\pi} \langle \{m_l\}, k|\langle \{m_l\}, k|dk.
$$

(60)

As $\hat{N}$ corresponds to $\hat{x}^{(N)}_d$ in section III, the same steps as in calculation of $[\hat{x}^{(N)}_d, \hat{k}^{(N)}_b]$ lead to

$$
[\hat{N}, \hat{k}] = i \left(1 - 2\pi \sum_{\{m_l\}} \langle \{m_l\}, k = \pi|\langle \{m_l\}, k = \pi\rangle \right),
$$

(61)

which differs from what is usually assumed by the second term on the rhs.

V. IMPLICATIONS

Here we want to discuss if the subtleties in the definitions of the $\hat{k}$ operators and their non-canonical commutation relations have practical implications. We begin with the case of a Bloch electron in a homogenous field. Let us first summarize the main results presented in sections II and III. The well known fact that an initial state in the form of a linear combination of Bloch states with different band indices but the same value of $k$ remains in such a form with a sharp value of $k$, was expressed as $P_k(t) = P_{k-\epsilon t/\hbar}(0)$ (Eq. (24)). But in contrast to common belief this does not lead to Newton’s law in the form of Eq. (1) if $k(t)$ is interpreted as the expectation value of the linear operator $\hat{k}_b(t)$ with $\hat{k}_b$ defined in Eq. (34). The property usually not correctly taken care of is the periodicity in the reciprocal lattice of the operator $P_k$ (Eqs. (22) or (34)). An obvious way to avoid contradictions is not to work with $\hat{k}_b$ at all, but take Eq. (24) as the basic result and use the translation operator $T_a$ only, e.g. in the form of Eq. (32) without introducing a $\hat{k}$ operator. We briefly show that this is a useful way to proceed in the single band case. The Hamiltonian $\hat{H}_0$ can be expressed in terms of $T^{(1)}_a$

$$
\hat{H}_0 = \sum_{n>0} \left( \epsilon_{n,0} (T^{(1)}_a)^n + h.c. \right),
$$

(62)

where the $\epsilon_{n,0}$ are the hopping matrix elements. In the following we drop the superscript (1) at the single band translation operator $T^{(1)}_a$. Its representation in Eq. (32) easily leads to the commutation relation $[\hat{x}, T^{(n)}_a] = na\hat{T}^{(n)}_a$, where $\hat{x} \equiv \hat{x}^{(1)}$. Therefore the Heisenberg equation of motion for $\hat{x}(t)$ reads

$$
i\hbar \dot{\hat{x}}(t) = a \sum_{n>0} \left( n\epsilon_{n,0} T^{(n)}_a(t) - h.c. \right).
$$

(63)

With Eq. (4) its solution can be found by integrating from 0 to $t$

$$
\hat{x}(t) - \hat{x} = \sum_{n>0} \left[ \epsilon_{n,0} T^{(n)}_a \left( e^{-in\epsilon t/\hbar} - 1 \right) / F + h.c. \right].
$$

(64)
If one takes an arbitrary wave packet as an initial state the expectation value of $\hat{B}/-\Delta$ shows periodic behaviour with time $T = 2\pi\hbar/aF$, the well known Bloch oscillations. For the case of nearest neighbour hopping the expectation value of $\hat{T}_{e}$ determines the amplitude of the oscillation. If the wave packet is well localized in $k$-space the amplitude is given by $B/2F$, where $B$ is the band width, while a Wannier-Stark eigenstate $|E\rangle$ or a Wannier state $|m\rangle$ as an initial state lead to zero amplitude of the Bloch oscillation. For the former all expectations are time independent, while the Wannier state behaves similar to a squeezed state with a periodic modulation of $\langle (\delta \hat{x}(t))^2 \rangle$. Note that for this description of the $N = 1$ case no $k$-operator was needed. For $N > 1$ the Wannier states are luckier for this “fixed point model” of interacting fermions in one dimension. If backscattering or impurity scattering are included the Hamiltonian has additional terms which are not of the simple form of Eq. (65). If one wants e.g. to evaluate the partition function for a Hamiltonian $\hat{H} + \lambda \hat{D}'$ the expression in perturbation theory to all orders in $\lambda$ involves correlation functions for the system described by $\hat{H}$ defined in Eq. (65). The arguments just presented show that in this case the use of the wrong commutation relation does not lead to incorrect results. Nevertheless the example presented shows that the widely accepted use of the wrong commutation relation between the phase and the particle number operator requires proper care.

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APPENDIX A:

In this appendix we present the simple proof of Eq. (22) which states that the operators $\hat{P}_{k}$ originally defined in terms of plane wave states also have a simple representation in terms of Bloch states of an arbitrary periodic potential. In the proof we use the well-known identity

$$\sum_{m=-\infty}^{\infty} e^{imu} = 2\pi \sum_{l=-\infty}^{\infty} \delta(u + 2\pi l) \equiv 2\pi \delta_{2\pi}(u),$$

where the index “$2\pi$” indicates the $2\pi$-periodicity of the argument of the delta function. We use this relation to show how $\hat{P}_{k}$ acts in the position representation.
For a Bloch state \( |k', \alpha \rangle \) Bloch’s theorem \( \langle x - am|k', \alpha \rangle = e^{-ik'am}(x'|k', \alpha) \) in Eq. (A2) yields, again using Eq. (A1)

\[
\langle x|\hat{P}_k|k', \alpha \rangle = \frac{a}{2\pi} \sum_{m=-\infty}^{\infty} e^{ikam} \psi(x - am).
\]

(A2)

If we define the operator \( \hat{P}_k = \sum_{\beta}|k, \beta\rangle \langle k, \beta| \) the matrix elements \( \langle x|\hat{P}_k|k', \alpha \rangle \) follow immediately as

\[
\langle x|\hat{P}_k|k', \alpha \rangle = \delta_{2\pi/a}(k - k')\langle x'|k', \alpha \rangle.
\]

(A3)

As \( \langle x \rangle \) and \( |k', \alpha \rangle \) in Eqs. (A3) and (A4) are arbitrary this proves \( \hat{P}_k = \hat{P}_k \), i.e. Eq. (22).

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1. C. Kittel, *Introduction to Solid State Physics* (John Wiley, New York, 1967)
2. N. Ashcroft and D. Mermin *Solid State Physics* (Holt & Rice, New York, 1976)
3. C. Kittel, *Quantum Theory of Solids* (John Wiley, New York, 1963)
4. J. Callaway, *Quantum Theory of the Solid State, Part B* (Academic, New York, 1974)
5. J.E. Avron, Ann. Phys. (N.Y.) 143, 33 (1982)
6. G. Nenciu, Rev. Mod. Phys. 63, 91 (1991)
7. G.H. Wannier, Phys. Rev. 117, 1366 (1960)
8. J.B. Krieger and G.J. Iadrate, Phys. Rev. B33, 5494 (1986)
9. D. Judge, Phys. Lett. 5, 189 (1966)
10. K. Kraus, Z. Phys. 188, 374 (1965) and unpublished notes
11. H. Kroemer, Am. J. Phys. 54, 177 (1986)
12. F.D.M. Haldane, J. Phys. C14, 2585 (1981)
13. A.O. Gogolin, A.A. Nersesyan and A. M. Tsvelik, *Bosonization and strongly correlated systems* (Cambridge University Press, 1998)
14. J. von Delft and H. Schoeller, Ann. Phys. (Leipzig) 7, 225 (1998)
15. K. Schönhammer, “Interacting Fermions in one dimension: The Tomonaga-Luttinger model”, cond-mat/ 9710330.
16. K. Schönhammer and V. Meden, Am. J. Phys. 64, 1168 (1996)
17. Were the “usual” argument fails can be most clearly seen in Ref. 4, where a discussion of the general solution \( |\psi(t)\rangle \) of the time dependent Schrödinger equation in the homogeneous external field is given. The author fails to take into account that \( \sum_{\alpha} \langle k, \alpha|\psi(t)\rangle |^2 \) is a periodic function of \( k \) in his calculation of \( \langle k \rangle \).