

## Interaction-induced oscillations in correlated electron transport

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The correlated motion of electrons in a one-dimensional system with an externally applied longitudinal electric field is discussed. Within the tight-binding model we show that in addition to the well-known Bloch oscillations, the electron-electron interaction induces time-dependent oscillations of the mobility whose period depends on the strength and range of the coupling only. The oscillations involve transitions between bands of bound and unbound states. The case of two electrons is solved in detail and an extension of the results to more particles is discussed.

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There has been much interest recently in nanostructures containing very few electrons, the entrance or exit of which can be controlled by a gate voltage.<sup>1</sup> While transport properties in these devices have been well studied and understood within independent electron approximations or mean-field theories, the effect of correlations is still largely unresolved.<sup>2,3</sup> An important question concerns the effect of the electron-electron interaction on the localization induced by disorder, a subject of recent controversy.<sup>4-12</sup> The usual approach to deal with this problem is to look for approximate solutions or estimates of unperturbed properties of the system, such as the decay rate of the ground-state localized wave functions. We here take a different route, and treat explicitly the time-dependent response of the ensemble to an external uniform electric field, in order to judge the ability to conduct through a study of the mobility. Our main finding is that this quantity oscillates in time with a period solely determined by the strength and range of the interaction.

The simplest case to treat is that of just two interacting electrons. We consider first such a pair, constrained to a one-dimensional chain of lattice parameter  $a$ , with an electric field  $\mathbf{F}$  applied along the wire. In the tight-binding model, the amplitudes  $C_{l,m}$  for having one particle at site  $l$  and the other at site  $m$  at time  $t$  obey the equation

$$\begin{aligned} & -\lambda(C_{l+1,m} + C_{l-1,m} + C_{l,m+1} + C_{l,m-1}) + E_{l,m}C_{l,m} \\ & = i\hbar \frac{dC_{l,m}}{dt}, \end{aligned} \quad (1)$$

where  $E_{l,m} = \epsilon_l + \epsilon_m + V(l-m) - eFa(l+m)$ , with  $\epsilon_l$  the energy at site  $l$  and  $V(l-m)$  the two-body interaction potential.  $\lambda$  is the usual hopping energy. In this model either of the two charges can hop to its nearest-neighbor site. Disorder may be included by making the site energies  $\epsilon_l$  random.

The two-electron problem described above is equivalent to that of a single particle moving in a square lattice with sites on the plane labeled by the pair  $l,m$ . The interaction acts like an interface potential, symmetric about the diagonal  $l=m$  where the boundary is located, and the applied external field is parallel to this line. The spectrum and eigenstates of the system with no electric field, no disorder, and a contact

Hubbard interaction  $V(l-m) = U\delta_{l,m}$  are easily found for this problem. To obtain the solution, we make in Eq. (1) the substitution

$$C_{l,m} = e^{i(l+m)ka} f(l-m) \quad (2)$$

in terms of new amplitudes  $f$  that depend on the distance  $u = l-m$  to the interface only. It is found that  $f$  obeys a one-dimensional equation, with hopping amplitude  $-2\lambda \cos(ka)$  and a chain of defects of local potential  $U$  along the line  $l=m$ , separating two identical media. The eigenstates bounded to this interface, which we shall call paired states, are then given by

$$f(l-m) = A e^{-\alpha|l-m|}, \quad (3)$$

$$E = \text{sgn}(U) \sqrt{U^2 + 16\lambda^2 \cos^2(ka)},$$

with  $A$  a normalizing constant, and  $\alpha = -\text{arcsinh}[U/4\lambda \cos(ka)]$ . The range  $\pi/2 < ka < 3\pi/2$  defines an energy band covering the interval  $U \leq E \leq \sqrt{U^2 + 16\lambda^2}$  for  $U > 0$ , while a symmetric band of negative energies appears for  $U < 0$  and  $-\pi/2 < ka < \pi/2$ . Note that the interaction gives more weight to configurations for which the electrons lie one on top of the other ( $l \approx m$ ), regardless of the sign of the interaction. Notice also that  $\alpha$  diverges at the lower edge of the  $U > 0$  band (upper edge of the  $U < 0$  band), leading to extreme localization with finite amplitudes along the interface  $l=m$  only. The wave function is symmetric under exchange of particles and is therefore appropriate to a singlet state. Together with this band of paired states there is also a band of pure plane-wave solutions covering the interval  $(-4\lambda, 4\lambda)$ , which correspond to traveling waves that scatter off the defect line  $l=m$ . The two bands giving paired and extended states overlap except for  $U > 4\lambda$ .

In discussing transport we consider the time-dependent average position  $\langle z \rangle = \sum_{l,m} P(l,m)(l+m)a$  in the linear chain, where  $P(l,m) = C_{l,m}^* C_{l,m}$  is the probability of finding one electron at site  $l$  and the other at site  $m$ . We then take the time derivative of this expression to find the velocity. After some algebraic manipulation we arrive with the use of Eq. (1) at the following expression for the average velocity, rigorous for the infinite chain,

$$\langle v \rangle = -\frac{2\lambda a}{\hbar} \text{Im} \sum_{l,m} C_{l,m} (C_{l+1,m}^* + C_{l,m+1}^*). \quad (4)$$

Exact results may be obtained in special cases with no disorder. For the paired states (3) in the absence of an external field the average velocity along the chain is a constant,

$$\langle v \rangle = \frac{2\lambda a}{\hbar} \frac{\sin(ka)}{\cosh \alpha}. \quad (5)$$

Note that the velocity is reduced by the interaction through the denominator in this expression. In the presence of the field but this time with no interaction the result is

$$\langle v \rangle = \frac{2\lambda a}{\hbar} \sin(ka + eFat/\hbar), \quad (6)$$

giving the well-known Bloch oscillations of period  $T_B = h/eFa$ .<sup>13-15</sup> The combined case with external field and interactions may be solved for  $\lambda \ll eFa$  by noting that in this limit

$$C_{l,m}(t) = C_{l,m}(0) e^{-(i/\hbar)E_{l,m}t} + O(\lambda), \quad (7)$$

so that owing to the presence of the external field, to the lowest order of approximation, the sites in the two-dimensional (2D) lattice acquire different time-dependent phases. From Eqs. (3), (4), and (7), one then obtains for the paired states the following result, to  $O(\lambda)$ :

$$\langle v \rangle = \frac{2\lambda a}{\hbar} \sin\left(ka + \frac{eFat}{\hbar}\right) \frac{\left(1 - 2(1 - e^{-2\alpha}) \sin^2 \frac{Ut}{2\hbar}\right)}{\cosh \alpha}. \quad (8)$$

Note that the drift velocity is again decreased by the interaction through the denominator in this expression, tending to zero as one approaches the bottom of the band ( $ka = \pi/2$  for  $U > 0$ ,  $ka = 0$  for  $U < 0$ ). The result also shows that the coupling introduces an oscillation of period  $T_I = h/U$ . Although the amplitude of this interaction induced oscillation (ININO) depends on the hopping amplitude  $\lambda$ , its period is independent of this quantity and depends only on the interaction strength  $U$ .

A more general result for any form of the interaction potential may be obtained if one assumes that the system is in a plane-wave (Bloch) state at  $t=0$ . Using Eqs. (4) and (7) and ignoring disorder one then gets, to  $O(\lambda)$ ,

$$\langle v \rangle = \frac{2\lambda a}{\hbar} \sin\left(ka + \frac{eFat}{\hbar}\right) \frac{1}{N^2} \sum_{l,m} \cos\left(\frac{\delta V_{l,m}t}{\hbar}\right). \quad (9)$$

Here  $N$  is the number of sites and  $\delta V_{l,m} = V(l+1-m) - V(l-m)$ . The sum in this expression is bounded from above to  $N^2$  adding evidence that the interaction in general reduces the drift velocity. Also, for the contact-interaction model only  $\delta V_{l,m} = U$  occurs in the argument of the cosine when finite, so that, as in Eq. (8), there is an oscillation of period  $T_I = h/U$ . For a long-range interaction several frequencies may be present, however.

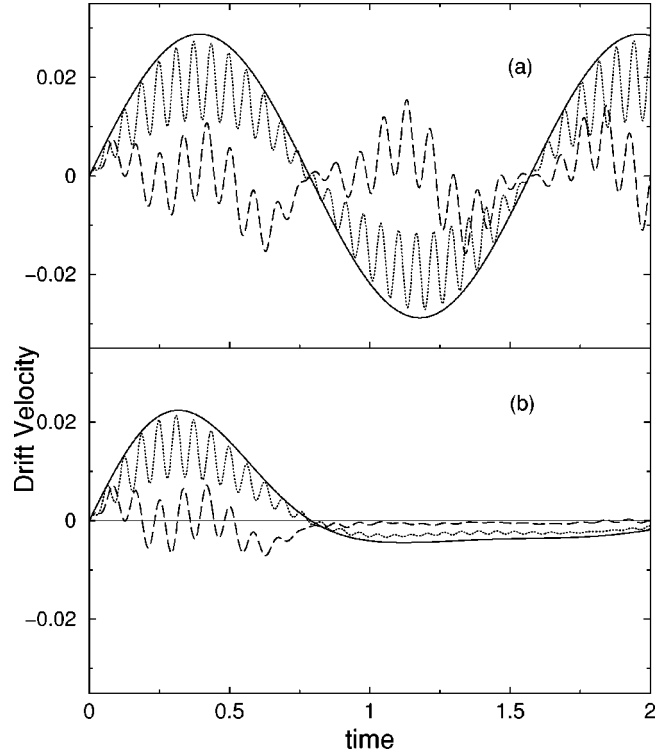


FIG. 1. Center-of-mass drift velocity for a pair of electrons in an electric field, without (a) and with (b) disorder. The dotted (full) line is the evolution with (without) a contact interaction. The dashed line includes a contact potential as well as a Coulomb tail. For details see text.

Next we consider disorder. From Eqs. (4) and (7) it is easy to see that the contribution of a disordered distribution of site energies appears through phase factors of the form  $\exp[i(\epsilon_{l+1} - \epsilon_l)t/\hbar]$ , so that the average over disorder yields an overall factor  $\langle \langle \cos[(\epsilon_{l+1} - \epsilon_l)t/\hbar] \rangle \rangle$  in the drift velocity (4), which at all times is less than 1. Thus, disorder decreases the drift velocity of the pair without affecting the period of the interaction-induced oscillation discussed above.

Up to now our results rely on approximation (7) that holds when  $\lambda \ll eFa$ . We have performed numerical calculations to test all ranges of parameters. A sample of our results is shown in Figs. 1 and 2. The units of distance and time are  $a$  and  $\hbar/\lambda$ , respectively. In Fig. 1 we plot the time evolution of the center-of-mass drift velocity for  $eFa = 4\lambda$  without [Fig. 1(a)] and with [Fig. 1(b)] disorder, the latter included through a random diagonal energy distribution in the interval  $-5\lambda < \epsilon_l < 5\lambda$ . The solid line represents the Bloch oscillation with no electron-electron interaction, while the dotted curve is for the contact-interaction model with  $U = 100\lambda$ . The dashed line adds to the same contact interaction a Coulomb tail  $V_0/|l-m|$  with  $V_0 = U/4$ . Note first that, as exhibited by Eq. (8), the interaction reduces the velocity. Note also that the ININO's are clearly exhibited. They have a regular period, and as anticipated in the above discussion, more than one frequency is present in the long-range interaction model. A Fourier analysis of the data shows a strong ININO component redshifted by a factor of about 0.8. The initial conditions for this data were finite uniform amplitudes in the

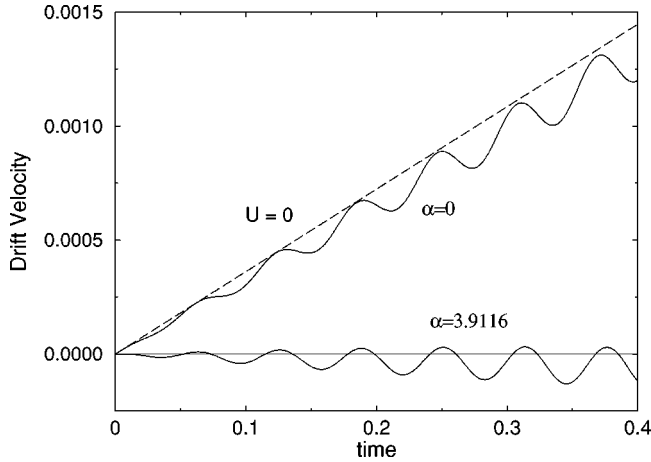


FIG. 2. Drift velocity for an interacting pair initially in a finite square on the  $l, m$  plane, with 11 sites on the side (full line labeled  $\alpha=0$ ). The case  $\alpha=3.9116$  has initial amplitudes as given by Eq. (3). The dashed line is the noninteracting case.

square  $-M < l \pm m < M$  with  $M=3$ , and zero amplitude elsewhere. The sample was a square lattice with up to 150 sites on each side, enough to avoid significant reflections from the edges within the time of computation. Increasing the size of  $M$  alters the relative amplitude of the oscillations without modifying the period. Note that disorder does not destroy entirely the ININO's although there is an overall reduction in the velocity that becomes more severe as time progresses.

Figure 2 shows the low-field case  $eFa=0.1\lambda$ ,  $M=10$ , and same value of  $U$  as above. Note that for these values of parameters in one Bloch oscillation one expects a thousand ININO periods, only the first few of which are shown. The almost perfectly straight (dashed) line is the noninteracting result, bounding from above the correlated case obtained for a uniform initial distribution, marked as  $\alpha=0$ . The curve labeled  $\alpha=3.9116$  was obtained with an initial paired state as given by Eq. (3) with  $ka=0$ . A different choice of  $k$  just introduces a phase shift and decreases the amplitude of the modulation, without affecting the period. The results exhibited show that, as apparent from Eq. (8), for this rather large value of the parameter  $\alpha$  the state is dominated by the ININO and motion is relatively slow. In this figure we chose to display a case with small external field in order to illustrate our finding that the ININO's exist away from the limit in which Eqs. (8) and (9) hold as well. Note that in spite of the diversity of initial conditions tested the oscillations are always present.

The above results are for two electrons. The spectrum then includes two relevant bands, one of extended states and one of bound states an energy  $U$  away, in which the electrons tend to be on top of each other as described by Eq. (3). The general case of  $N$  electrons may be treated in a similar way as we did for two particles, resorting now to the equivalent problem of a single electron in  $N$  dimensions with planar interfaces representing the interaction. For instance, if  $N=3$  one treats an electron in three dimensions  $m, l, n$ , with uniform defect sheets along the planes  $m=l$ ,  $m=n$ ,  $n=l$  and an electric field along the diagonal  $m=l=n$  where the

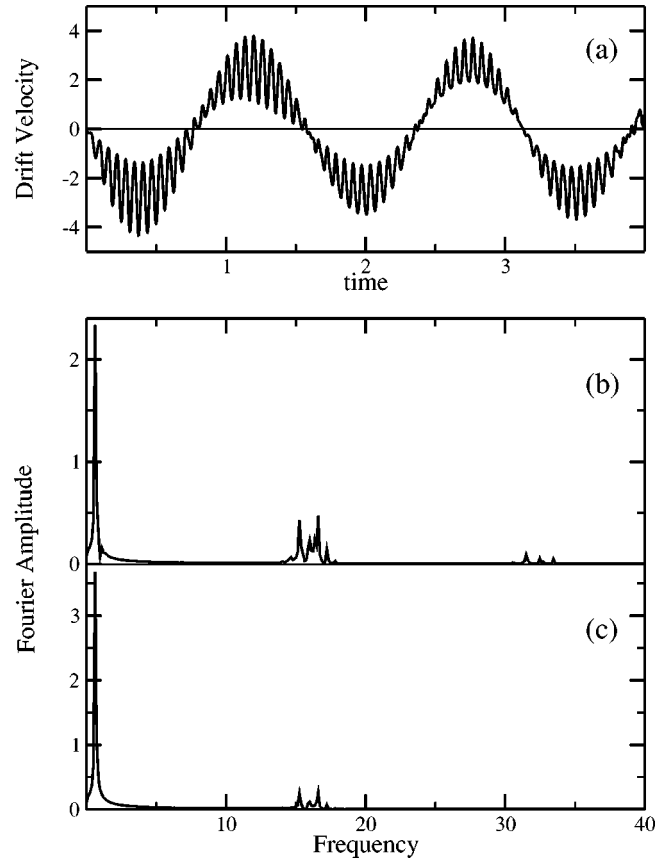


FIG. 3. Drift velocity (a), and spectral density for three interacting particles with finite initial amplitudes around the origin (b) and around the point  $(0,0,20)$  (c). Parameters are as in Fig. 1(a).

defect planes meet. Besides the band of extended states there are now two additional bands, one an energy  $\sim U$  away, associated with interface states (our so-called paired states), the other coming from states bound to the diagonal, an energy  $\sim 2U$  away (which we call tripled states). Figure 3(a) shows the center-of-mass velocity for this case using the same parameters as Fig. 1(a) with contact interaction only. Initially, the amplitudes are set finite only within a cube of side  $M=3$  around the origin  $(0,0,0)$ . The ININO oscillations are clearly present and, as shown in Fig. 3(b) where the spectral density is exhibited, include three main frequencies:  $eFa/\hbar$ ,  $U/\hbar$ , and  $2U/\hbar$ , representing the Bloch oscillations and transitions between the three bands. Notice that the weakest frequency is for oscillations involving the highest band. This is an important consequence of the reduced number of states in the interaction-induced upper bands. Figure 3(c) shows the spectral density for finite initial amplitudes over a similar cube as for Fig. 3(b) but surrounding the point  $(0,0,20)$ . Notice that this point is far from the diagonal  $m=l=n$  near which tripled states are localized so that no component in the highest band is expected. Indeed, the spectral density of the highest frequency  $2U/\hbar$  is negligible as is apparent in the figure. In the general case of  $N$  particles in a string of  $L$  sites the number of extended states equal about  $L^N$ , while the paired states number equal  $L^{N-1}$ , the tripled states  $L^{N-2}$ , the quadrupleds  $L^{N-3}$ , and so on. Thus the

amplitude of their contribution decreases in the same ratio and only the lowest of such bands is important. Then, a system with more than two particles will still exhibit the oscillations described. The equivalence of the 1D wire with  $N$  electrons and the motion of a single particle in  $N$  dimensions emphasized above may also be useful in checking the effect we are reporting. For instance, the experimental probe could be either a 1D system with three electrons, or one electron moving in a 3D lattice hosting a thin sheet of impurities.

In summary, we have shown that the electron-electron interaction induces a kind of oscillations in the drift velocity of electrons moving along a chain and subject to an external electric field, with a period determined solely by the interaction range and strength. The  $N$ -particle problem is identical to that of a single particle moving in an  $N$ -dimensional lattice, with defect surfaces dividing the space in symmetric domains. One can take advantage of the equivalence of the two cases to understand the physical origin of the oscillations. With no interactions the single particle in  $N$  dimen-

sions will respond to an external field purely through Bloch oscillations in a band of extended states, Eq. (6). The defect boundary introduced by the coupling gives rise to separate bands of surface states localized along the line perpendicular to the surface, such that electrons may exhibit oscillations between the free- and bound-state bands. This interpretation is supported by our numerical results showing that the INNO's disappear if one starts with a state with finite amplitudes far from the defect line only. In fact, as the square around the origin in which amplitudes are initially finite in Fig. 2 is enlarged, the oscillation of the upper curve is flattened due to the larger component in the lower extended-states energy band of the initial state, while the oscillation in the lower curve remains. If  $U$  is negative so that the band of paired states becomes the lowest in energy, then this latter oscillation is the one damped out.

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