DYNAMIC LOCALIZATION OF A PARTICLE IN AN ELECTRIC FIELD VIEWED IN MOMENTUM SPACE: CONNECTION WITH BLOCH OSCILLATIONS

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A recent investigation has shown that the motion of a charged particle on a discrete lattice under the action of a time-dependent electric field can exhibit a peculiar phenomenon involving the dynamic localization of the particle whenever the magnitude and frequency of the applied field are in certain ratios to each other. The connection of this phenomenon to the familiar effect of Bloch oscillations is studied by exploring the phenomenon in momentum space.

When a dc electric field is applied to a charged particle moving in a perfectly periodic crystal at zero temperature, the particle executes ac motion. In other words, in the absence of scattering (from lattice imperfections or ion motions), a dc electric field produces an ac current rather than a dc current. This effect is well-known [1–3]. It can be understood easily by following the evolution either in momentum (k) space or in real space. If the particle initially occupies a k-state, the applied dc field causes the particle to move in k-space at a rate proportional to the field magnitude. As it approaches the edges of the Brillouin zone, its velocity is reduced as a result of Bragg reflection, and, when it crosses the zone edge, it reenters on the other side of the zone. The particle velocity increases and decreases periodically. The result is cyclic motion and the current is ac. This effect is identical in essence to the localization of a particle initially occupying a single site state – Wannier state – when under the action of a dc electric field. The field lifts the degeneracy of the site states and the consequent energy mismatch among the site states hinders the motion from the initially occupied site to its neighbours. The particle returns to the initally occupied site repeatedly and the mean-square displacement is bounded and periodic.

The above static localization effect is textbook knowledge [1]. We have recently reported [4] a new localization effect which occurs when the applied field is not dc but varies sinusoidally in time. We found that, if initially localized at a site, the particle will generally escape that site under the action of an applied ac field of magnitude $\mathscr{E}$ and frequency ω (as in the field-free case) except in those cases in which the ratio $\mathscr{E}/\omega$, where $\mathscr{E}=eEa/\hbar$, is a root of the ordinary Bessel function J_0. In these special isolated cases the particle finds itself localized (as in the dc field case). Here, and in the rest of this Letter, the lattice consedered is a one-dimensional infinite chain with intersite distance a, the charge on the particle is e, and the intersite matrix elements (overlap integrals), denoted by V below, are nearest-neighbour in character. A study of the connection of this new effect, which we have termed [4] "dynamic localization", to the better known static localization effect as viewed in k-space, and to the phenomenon of Bloch oscillations [1], forms the content of this Letter.

As explained in ref. [4], the hamiltonian of the particle is given by

$$H(t)=V\sum_m \{|m\rangle\langle m+1|+|m+1\rangle\langle m|\} -eEaf(t)\sum_m m\{|m\rangle\langle m|\}\,, \tag{1}$$

where $|m\rangle$ represents a Wannier state localized on lattice site m, and $f(t)$ describes the time-dependence of the electric field.

An immediate consequence of (1), which we will find useful in our investigations below, is the form of the velocity operator. Either by finding the commutator of the hamiltonian H with the position operator

$$x=\sum_m m|m\rangle\langle m| ,$$

or by working out the evolution as in ref. [4], it is straightforward to show that the velocity operator is given by $\sum_k v_k|k\rangle\langle k|$ with

$$v_k=2Va\sin[k-\mathscr{E}\eta(t)] , \tag{2}$$

where

$$\eta(t)=\int_0^t ds f(s) .$$

For no field applied, (2) yields the well-known formula for the velocity matrix element in a tight-binding chain. In the presence of the field, it describes the fact that an initial k-state remains a k-state under the action of the field [4], rate of change of k being given exactly by $\mathscr{E}f(t)$.

The key to the understanding of the dynamic localization effect in k-space and of its connection to Bloch oscillations lies in the result that $\langle m^2\rangle$, the mean-square-displacement on an initially localized particle, is given by the sum over all the k-states in the Brillouin zone, of the square of a quantity m_k which may be regarded as the contribution of the state $|k\rangle$ to the particle displacement:

$$\langle m^2\rangle=\sum_k (m_k)^2 , \tag{3}$$

$$m_k=\int_0^t ds\, v_k(s)=\int_0^t ds\, 2Va\sin[k-\mathscr{E}\eta(s)] . \tag{4}$$

The proof of this results follows trivially on writing the mean-square-displacement for arbitrary initial conditions in the familiar form (see, e.g., eq. (2.5) of ref. [5]) as the double time integral of the velocity correlation function, using the fact that the initially localized condition allows the reduction of the general expression to

$$\langle m^2\rangle=\int_0^t\int_0^t dt_1\, dt_2\, \mathrm{Tr}\, v(t_1)v(t_2)$$

$$=\int_0^t\int_0^t dt_1\, dt_2 \sum_k \langle k|v(t_1)v(t_2)|k\rangle , \tag{5}$$

and realizing from (2) that $v(t_1)$ and $v(t_2)$ are diagonal in the k-representation.

Returning to (3) and (4), we see that localization, which corresponds to $\langle m^2\rangle$ being bounded, will occur whenever the contribution m_k to the particle displacement is bounded for every k-state in the band. An alternative way of expressing this statement is that the occurrence of localization implies that the time average (or time integral) of v_k, the velocity in the k-state, must vanish for every k. Using (2), we write v_k explicitly as

$$(1/2Va)v_k=\sin k\cos[\mathscr{E}\eta(t)]$$
$$-\cos k\sin[\mathscr{E}\eta(t)] , \tag{6}$$

and observe that, when the applied field is sinusoidal, $f(t)=\cos\omega t$, $\eta(t)$ is given by $(1/\omega)\sin\omega t$, and the cosine and sine functions multiplying $\sin k$ and $\cos k$ respectively in (6) may be expanded in terms of Bessel functions as

$$\cos[(\mathscr{E}/\omega)\sin\omega t]$$
$$=J_0(\mathscr{E}/\omega)+2\sum_p J_{2p}(\mathscr{E}/\omega)\cos(2p\omega t) , \tag{7}$$

$$\sin[(\mathscr{E}/\omega)\sin\omega t]$$
$$=2\sum_p J_{2p-1}(\mathscr{E}/\omega)\cos[(2p-1)\omega t] . \tag{8}$$

The p-summations in (7) and (8) run from 1 to ∞. With the exception of $J_0(\mathscr{E}/\omega)$, all the terms on the right-hand sides of (7) and (8) oscillate around a zero average value.

Eqs. (6)–(8) show that the average of the velocity v_k will vanish when and only when the term $J_0(\mathscr{E}/\omega)$ in (7) vanishes, i.e. whenever the ratio $\mathscr{E}/\omega$ takes on values equal to the roots of J_0. In all other cases, the constant term in the expansion (7) of

$$\cos[(\mathscr{E}/\omega)\sin\omega t]$$

will make m_k and the mean-square-displacement unbounded – as a result of the integration shown in (4) and (5) – and the particle will escape. This analysis shows that dynamic localization in a perfect crystal may be understood in k-space as arising whenever the average velocity in every k-state vanishes as a result of the particular form of the dispersion relation in the band and the time-dependence of the applied field. This is the primary result of this Letter.

The above reasoning and eq. (6) may also be applied to two simpler cases. The first is the static localization case when the applied field is constant in time. The function $\eta(t)$ is now t, both the cosine and sine terms in (6) average to zero, the average of the velocity in every k-state vanishes and the particle is localized no matter what the magnitude of the applied field is (with only the requirement that it not vanish). In this case, if the particle were to start from a specific k-state, it would traverse the entire Brillouin zone and sample all k-states. The periodicity of the band energy and therefore of v_k ensures that the average of v_k is zero and that there is localization.

The second case which is instructive to analyze with (6) is one in which the applied field follows a square wave, i.e. one which is constant in magnitude but whose sign is reversed every π/ω seconds. For this case $f(t)$ changes from 1 to -1 repeatedly, and $\eta(t)$ is a saw-tooth curve. The changes result in a function with a non-vanishing time average except if the following condition holds:

$$\mathscr{E}/\omega = 2, 4, 6, \ldots . \qquad (9)$$

If (9) holds, the motion of the particle in the Brillouin zone proceeds under a perfect synchronization of the Bloch oscillations characteristic of a constant (dc) field and the sign reversals of the field. The result is dynamic localization.

The study of the above case of a square-wave applied field makes quite clear the phenomenon of dynamic localization as viewed in k-space and its connection with Bloch oscillations. For the square-wave field, dynamic localization occurs whenever the time-dependence of the applied field is such that one or more *complete* Bloch oscillations are allowed to take place in exactly half the period of the field. For the sinusoidal field, the average of the magnitude of the field is less than in the square-wave case. Consequently the value of $\mathscr{E}/\omega$ has to be larger than in (9). Indeed, writing down the roots of the Bessel function explicitly we see that, for the sinuoidal field, (9) is to be replaced with

$$\mathscr{E}/\omega = 2.405, 5.520, 8.654, \ldots . \qquad (10)$$

We stress in closing that dynamic localization in the strictest sense will occur for a sinusoidal time-dependent applied field only for a tight-binding chain, i.e. for a sinusoidal dispersion relation. However, the physical effect of a lowering of the mobility as the ratio of the magnitude of the field to its frequency approaches certain values will be present in all cases.

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References

[1] P.W. Anderson, Concepts in solids (Benjamin, New York, 1963).
[2] M. Luban, J. Math. Phys. 26 (1985) 2386.
[3] J.B. Krieger and G.J. Iafrate, Phys. Rev. B 33 (1986) 5494.
[4] D.H. Dunlap and V.M. Kenkre, Phys. Rev. B 34 (1986) 3625.
[5] V.M. Kenkre, R. Kuehne and P. Reineker, Z. Phys. B 41 (1981) 181.
[6] H. Scher and M. Lax, Phys. Rev. B 7 (1973) 4491.