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Stark-Wannier states in disordered systems

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We compare numerical results on metastable Stark-Wannier states in two semi-infinite disordered Kronig-Penney models in the presence of an electric field with an analytic derivation from a WKB-Lyapunov–type formula. Results suggest vanishing of the width of the resonances at the infinite-system limit.

It is now clear that narrow resonances forming a quasi-ladder exist for some models which represent one-dimensional finite crystals in the presence of an external field; it is also a fact that the resonance widths exhibit, as the crystal is enlarged, large and unpredictable oscillations.[1,2] So it was not clear whether or not the resonance widths vanish in the infinite-crystal limit as suggested by Berezhkovskii and Ovchinnikov.[3] It appeared to us that by destroying the crystal regularity, the interference phenomena which cause the oscillations would disappear. Therefore we decided to address the limit problem for disordered systems. These systems are interesting on their own, because, due to the link between resonance widths, transmission coefficient, and resistance through Landauer-type formulas, their study can provide a better understanding of the resistance properties at low temperatures of thin wires like those made of doped semiconductors. Their interest comes also from the fact that a transition from localized to extended states at a positive field value has been observed by Soukoulis, José, Economou, and Ping Sheng[4] and proved in different situations by Prigodin[5] and Delyon and coworkers.[6]

We study two Schrödinger equations,[7]

$$\left(-\frac{d^2}{dx^2}+\sum_{n=-N_0}^{N} V_n\delta(x-n) -F\sum_{n=-N_c}^{N}\Theta(x-n)+FN_0\right)\psi(x)=E\psi(x) \quad , \tag{1}$$

which differ by the distribution of the mutually independent random variables V_n. In model I the V_n distribution is uniform in a symmetric interval $[-\sqrt{12},\sqrt{12}]$ exactly as in Ref. 4, while in model II, we introduce a "less disordered" distribution (not considered in Refs. 4 and 6) uniform in $[-3,-1]$.

Equation (1) can be easily transformed into the finite-difference system:

$$\begin{pmatrix}\psi_n\\ \psi_n'\end{pmatrix}=\begin{pmatrix}c_n & s_n\\ V_nc_n-k_n^2s_n & V_ns_n+c_n\end{pmatrix}\begin{pmatrix}\psi_{n-1}\\ \psi_{n-1}'\end{pmatrix} \quad , \tag{2}$$

where $c_n=\cos k_n$, $s_n=k_n^{-1}\sin k_n$; $k_n^2=E+Fn$ is the effective energy at n; $\psi_n=\psi(n)$, $\psi_n'=\psi'(n^+)$.

Resonances are defined as usual[2,8] by the Sommerfeld condition at N^+, $\psi_N'=ik_N\psi_N$ with $\psi_N=1$, and the L^2 condition at $-\infty$ is given by $\psi'_{-N_0-1}=|k_{-N_0-1}|\psi_{-N_0-1}$.[9] Actually the research of resonances is made easier by previous computation of bound states with the boundary condition $\psi_N=0$.

We remark that resonances are so narrow that corresponding wave functions have the same behavior as any wave function corresponding to a nearby real energy whatever the initial condition at N. Numerical computations give the following generic decrease for $E\simeq 0$:

$$\ln(\psi_n^2+\psi_{n+1}^2)\sim C_0+C_1\ln(Fn) \quad \text{as } n\to+\infty \tag{3}$$

with superimposed regular oscillations of period π in the $(Fn)^{1/2}$ variable, apparently almost constant (see Fig. 1) and independent of F. C_1 is apparently linear in F^{-1} in the range [0.125,4.0]

$$C_1(F)=0.5+(1\pm0.1)F^{-1} \quad \text{for model I} \quad , \tag{4}$$

$$C_1(F)=0.5+(1.1\pm0.3)F^{-1} \quad \text{for model II} \quad . \tag{5}$$

If we define as critical field F_c the value for which we pass from extended to localized L^2 wave functions, we get, for model I, $F_c\simeq 2$ and, for model II, $F_c\simeq 2.2$. If we compare with Ref. 4 our definition coincides with their $F_c^{(3)}$ definition and our critical value in model I corresponds to their $F_c^{(2)}$ value.

Their heuristic explanation can be made more precise using a WKB-Lyapunov–type formula. An equivalent form of (2) is

$$\psi_{n+1}+\frac{k_n}{k_{n+1}}\frac{\sin k_{n+1}}{\sin k_n}\psi_{n-1}-\left(V_n\frac{\sin k_{n+1}}{k_{n+1}}+\cos k_{n+1}+\frac{k_n}{k_{n+1}}\frac{\sin k_{n+1}}{\sin k_n}\cos k_n\right)\psi_n=0 \quad . \tag{6}$$

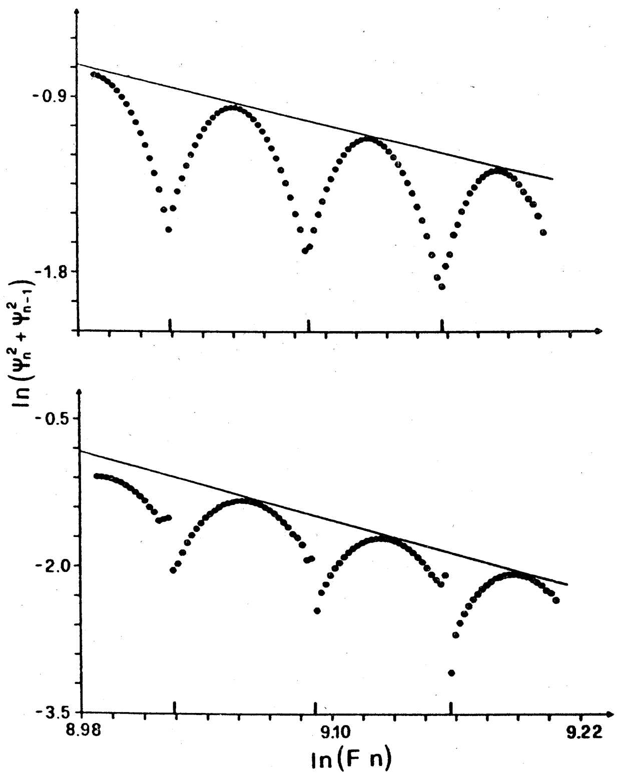

FIG. 1. Behavior of the wave function ψ_n for $E=0$ (mean is over 6000 samples). Top: model I, with $F=0.5$. The slope of the line drawn here is -2.5. Bottom: model II with $F=0.25$. The slope of the line drawn here is -5.75.

For $F=0$ we get

$$\psi_{n+1}+\psi_{n-1}-\left[V_n\frac{\sin\sqrt{E}}{\sqrt{E}}+2\cos\sqrt{E}\right]\psi_n=0 \tag{7}$$

whose solutions behave like

$$\psi_n\sim\exp[\pm\alpha(E)n] \quad \text{as } n\to\infty \ , \tag{8}$$

with $\alpha(E)=\gamma(E)+iK(E)$. [$\gamma(E)$ is the Lyapunov exponent; $K(E)$ is the rotation number which describes the number of changes of sign of the solution per unit length and is equal to the integrated density of states.[6(b)]]

We observe that (6) can be mainly recovered from (7) if in this latter E is replaced by $E+Fn$. As $\alpha(E+Fn)$ plays the role of the wave vector $k(E,x)=[E-V(x)]^{1/2}$ in ordinary WKB formulation we look for a solution of the form

$$\psi_n=A_n\exp\left[\pm\sum_{j=1}^{n}\alpha(E+Fj)\right] \ .$$

Inserting it in (6) and considering (8) as the solution of (7), and not only as its asymptotic form, we get

$$\psi_n\sim\frac{1}{[\alpha(E+Fn)]^{1/2}}\exp\left[\pm\sum_{j=1}^{n}\alpha(E+Fj)\right] \quad \text{as } n\to+\infty \ . \tag{9}$$

Now we only need to calculate the expressions of γ and K.

For model I, we compare (7) and the tight-binding (TB) Anderson model for disordered systems:

$$\psi_n+\psi_{n-1}+V_n\psi_n=E\psi_n \ .$$

If γ_{TB} and K_{TB} denote the Lyapunov exponent and the density of states for this latter, we get

$$\begin{aligned}\gamma(E,W)&=\gamma_{TB}(E_{TB},W_{TB}),\\ K(E,W)&=K_{TB}(E_{TB},W_{TB})\ ,\end{aligned} \tag{10}$$

with $E_{TB}=2\cos\sqrt{E}$, $W_{TB}=W(\sin\sqrt{E})/\sqrt{E}$.

To take into account the main features of γ_{TB} (except the anomalies,[10,11] which in fact could be treated in a similar way) we consider on a heuristic standpoint

$$\gamma_{TB}^{-1}(E_{TB},W_{TB})\sim W_{TB}^{-2}[24(4-E_{TB}^2)+O(W_{TB}^{4/3})] \quad \text{as } W_{TB}\to 0 \ , \tag{11}$$

which combines the Thouless approximation[12] near the band center and the Derrida-Gardner formula[10] at the band edge. Despite the fact $\gamma(E_n,W)=0$, $E_n=n^2\pi^2$, from Eq. (11) it is easy to prove that $\gamma(E,W)$ is substantially smaller than $(W^2/96)E$ only in intervals $|E-E_n|<C$, $C>0$, so that

$$\sum_{j=1}^{n}\gamma(E+Fj)\sim(W^2/96)\ln(E+Fn) \quad \text{as } n\to+\infty \ .$$

Similarly, to calculate

$$K(E,W)\equiv\int_{-\infty}^{E}\rho(E',W)dE'$$

we start with the heuristic behavior for the tight-binding

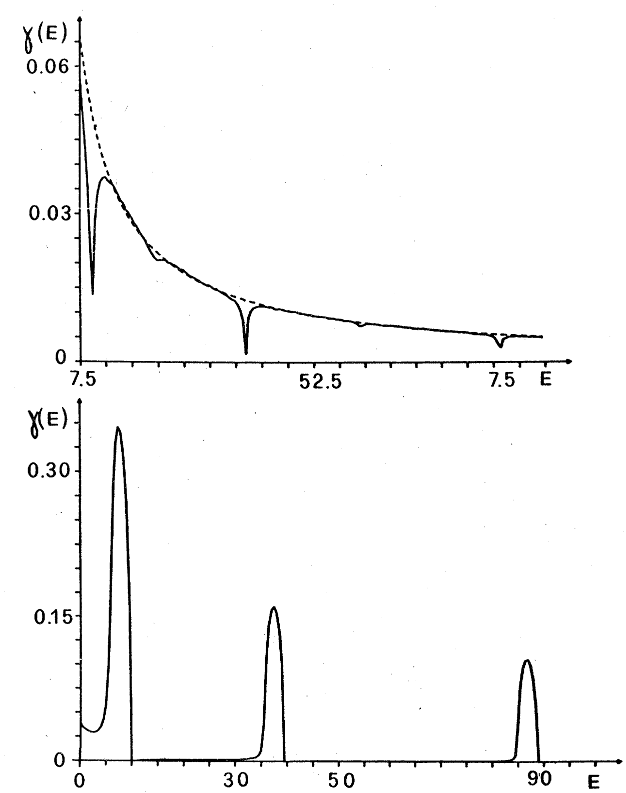

FIG. 2. Lyapunov exponent for the Kronig-Penney models ($F=0$). Top, model I; bottom, model II.

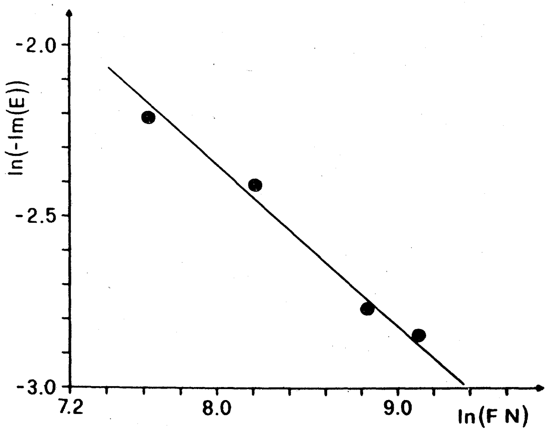

FIG. 3. Resonance width behavior for model I with $F=8$.

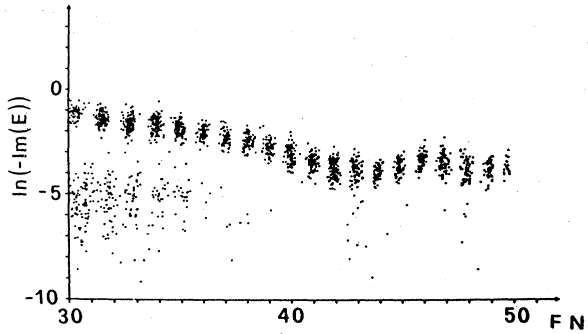

FIG. 4. Ladder structure (model II, $F=1$) for resonances whose $|\psi_n|$ has a maximum at some point $\bar{n}$ with $\mathrm{Re}E+\bar{n}F$ in the second band: $[\pi^2, 4\pi^2]$.

density of states

$$\rho_{\mathrm{TB}}(E_{\mathrm{TB}}, W_{\mathrm{TB}}) \sim 1/[4\pi(1-E_{\mathrm{TB}}^2)^{1/2}+O(W_{\mathrm{TB}}^{2/3})] \quad \text{as } W_{\mathrm{TB}} \to 0 \;.$$

Using formulas (10) we get $\rho(E,W) \sim 1/(4\pi\sqrt{E})$ as $E \to \infty$ if $|E-E_n| > C$. Then asymptotically $K(E,W)$ goes like $E^{1/2}$.

Inserting in (9) the estimates just above and letting $E=0$,

$$|\psi_n| \sim \frac{1}{(Fn)^{1/4}} e^{\pm (W^2/96F)\ln(Fn)} = (Fn)^{-1/4 \pm W^2/96F} \;.$$

Taking the minus sign we get perfect agreement with the numerical analysis given by (2) and (3).

The oscillations cannot be completely explained at this order of WKB approximation which makes the behavior monotonic. In any case, as $\alpha'(E+Fx)$ is singular at $x_n=(E_n-E)/F$, these points could be considered as turning points and large deviations from the WKB formula are expected there.

For model II we can see that $\gamma(E)$ is fairly well approximated (Fig. 2) by the Lyapunov exponent for the crystal $V_n=V=-2$. From this it can be seen that

$$\int_0^{Fn} \gamma(E)dE \simeq \sum_{l;E_l<Fn} \frac{V^2}{4l} \sim \ln[(Fn)^{1/2}/\pi] \quad \text{as } n \to \infty \;.$$

For similar considerations as for model I, $K(E)$ behaves like $\sqrt{E}$ as $E\to\infty$. From formula (9) we get $C_1(F)=0.5+F^{-1}$ in good agreement with (5).

Now we pass to consider the resonance widths. Note that instead of fixing N and to varying $\mathrm{Re}E$ as in Ref. 8 it is equivalent to look at resonances near 0 and to vary N, so FN plays the role of $\mathrm{Re}E$. Then by the well-known formula for the resonance width we get as $N\to\infty$

$$\mathrm{Im}E = \frac{\mathrm{Im}(\psi_N \bar{\psi}'_N)}{\int_{-\infty}^{N} |\psi(x)|^2 dx} \sim \begin{cases} (FN)^{-C_1(F)+0.5} = (FN)^{-F_c/2F} & \text{for } F<F_c, \\ (FN)^{-0.5} & \text{for } F \geq F_c, \end{cases}$$

in agreement with the numerical results (see Fig. 3).

For model II we observe the resonances are almost arranged in Wannier ladders as in crystals (Fig. 4). Here wave functions do not need to cross a "gap," as in the usual Zener effect[8] in order to give rise to narrow resonances.

It turns out that our results are compatible with the following conjecture: As the sample becomes infinite the resonances become bound states for $F<F_c$. For $F\geq F_c$ the width of the resonances do vanish and the "eigenfunctions" in the limit are characterized by the behavior

$$|\psi_N|^2 \sim N^{-F_c/2F-0.5} \quad \text{as } N\to\infty$$

(while the other possible behavior is $N^{F_c/2F-0.5}$). To study for $F\geq F_c$ the evolution of a wave packet it should be very interesting to know if this behavior is linked to some characterization of the operator spectrum.

We expect wave packets locally approximating Stark-Wannier states to be metastable in a sense to be specified.

Finally, from the similarity of model II and crystal models, in view, for instance, of the $\gamma(E)$ values, we can expect these results to be valid for crystals.

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