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Localization and level statistics in a one-dimensional solid state model with periodically modulated potential

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For a solid state model described by a band matrix with diagonal elements depending periodically on the site-index we determine the eigenstates and their localization length. The periodicity of the diagonal elements gives rise to the appearance of a pronounced peak structure of the eigenstates with the same period. The same type of peak-structure is present in the quasi-energy states of some periodically driven quantum systems, and can be associated with a nearly conversed quasi-momentum quantum number. We investigate the influence of the periodic peak structure on the nearest neighbor level spacing distribution and find that the nearly conserved quasi-momentum modifies but does not destroy the level repulsion expected for a Gaussian orthogonal ensemble.

1. Introduction

In disordered one-dimensional solids with short-range interaction Anderson localization is well known to occur [1], i.e. the energy spectrum is pure point and eigenstates are exponentially localized. The nearest neighbor level spacing distribution of a finite number of states shows level repulsion and follows the Gaussian orthogonal ensemble of random matrix theory if the states considered are neighbored within a localization length [2]. This distribution will be Poissonian and show no level repulsion if the spatial centers of the states are separated by much more than a localization length, since the energies of such states are completely independent. What happens if the amplitudes of the localized states within a localization length are confined to periodically spaced and narrow peaks? States with practically the same center of localization whose peaks are phase-shifted with respect to each other will then have very small overlap. Since these states do not 'feel' each other they should have a correspondingly suppressed level repulsion. The same suppression of the level repulsion one would also expect by the argument that the near-periodicity of the peak structure of the localized state, if strictly periodic, would be associated with a conserved quasi-momentum. Levels with different quasi-momentum would then be independent and would not repel each other.

The assumed peak substructure of the localized states is not as contrived as it might seem at first glance. It occurs naturally in localized quasi-energy states of periodically driven quantum systems if the number of unperturbed levels in these systems in the range of the external frequency ω (we put $\hbar=1$) is much larger than 1, that implies $\rho\omega\gg 1$, where ρ is the smoothed density of states [3]. These periodically driven quantum systems bear a close analogy to 1-dimensional solid state systems, as first demonstrated for the case of the periodically kicked rotator in [4]. In the present paper it is our purpose to introduce a 1-dimensional solid state model in which localized states with a periodic substructure can be expected to appear (Sect. 2), analyze the localized states of that model (Sect. 3) and find the nearest neighbor level spacing distribution (Sect. 4). Our results are briefly summarized in Sect. 5.

2. The model

Let us consider a 1-dimensional chain of periodic lattice-sites labelled by n and let the Hamiltonian be given by

$$H=\sum_n E_n|n\rangle\langle n|+\sum_{n,n'} V_{nn'}|n\rangle\langle n'| \tag{2.1}$$

We shall assume that the energy E_n on the lattice-sites varies periodically with n, with period $E_{n+M}=E_n$. A natural realization of this assumption would be a solid structure grown of epitaxial layers each of thickness M in the lattice constant. We shall assume $M\gg 1$, i.e. the number of lattice sites in one period is large. In our numerical work we choose

$$E_n=\frac{1}{\rho}\left(\left(n+\frac{M}{2}\right)(\mathrm{mod}\,M)-\frac{M}{2}\right)+\varepsilon_n \tag{2.2}$$

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where we normalized the energy scale so that $\rho=1$. The ε_n are random and will be specified later. The potential matrix $V_{nn'}$ in (2.1) is assumed to be a band matrix. We shall be interested in the transport in the periodic background described by the diagonal elements E_n from one period to its neighboring period and choose

$$V_{nn'}=\begin{cases} V & \text{if } \frac{M}{2}<|n-n'|<\frac{3M}{2} \\ 0 & \text{else} \end{cases} . \tag{2.3}$$

We make this choice in order to strengthen the analogy of our solid state model with periodically driven quantum systems. There, transitions between 'sites' (i.e. energy levels E_n) are caused by the absorption or emission of a photon. Therefore energy differences $|E_n-E_{n'}|$ of states coupled by $V_{nn'}$ naturally lie in some band around the 1-photon energy $\omega=M/\rho$ where ρ is the density of states [5]. We note, however, that the results will not change qualitatively if in (2.3) we replace the lower boundary of the band by 0. The choice of (2.3) has the added advantage that the model becomes closely related to a model for multi-photon excitation in molecular quasi-continua [6], which has analytically solvable limits with which we can compare our results. In that model (2.2) also holds and (2.3) is replaced by

$$V_{nn'}=V\delta_{m_n,m_{n'}} \tag{2.4}$$

where m_n is the integer closest to (E_n/M). This matrix consists of two lines of blocks of the size M next to the diagonal, while the matrix (2.3) consists of two bands of width M parallel to the diagonal at a distance M. In the case where the energy levels are not random, $\varepsilon_n=0$, the eigenstates are, of course, extended Bloch states and the energy eigenvalues are continuous.

If the ε_n are nonzero the Schrödinger equation has to be solved numerically. We have considered two cases:

i) ε_n is distributed randomly and independently for each n over the interval $(-\frac{1}{2}+n, \frac{1}{2}+n)$.
ii) The E_n are distributed on the real line as a discrete Poisson process with independent random increments in the interval [0, 2].

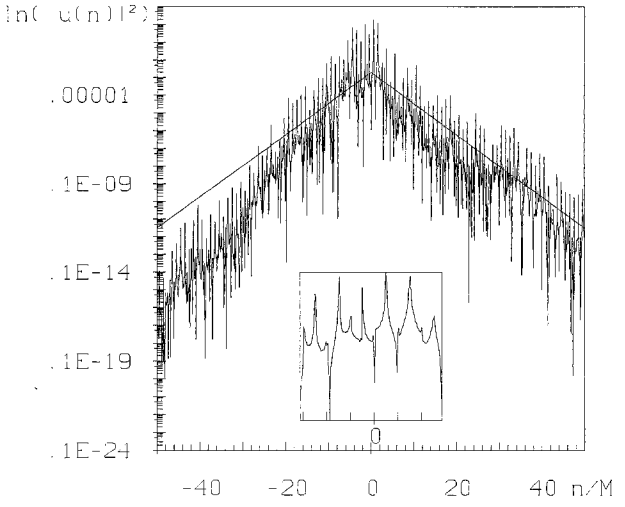

Fig. 1. Localized eigenstate for energy $E=0.471$ over distance measured in periodicity intervals. A part near the maximum is amplified in the insert, also in logarithmic scale. The straight lines give the exponential decay with the smallest eigenvalue of the transfer matrix. Parameters are $V=0.5$, $M=32$, $N=100$. $|u(n)|^2$ the probability of the unperturbed level E_n

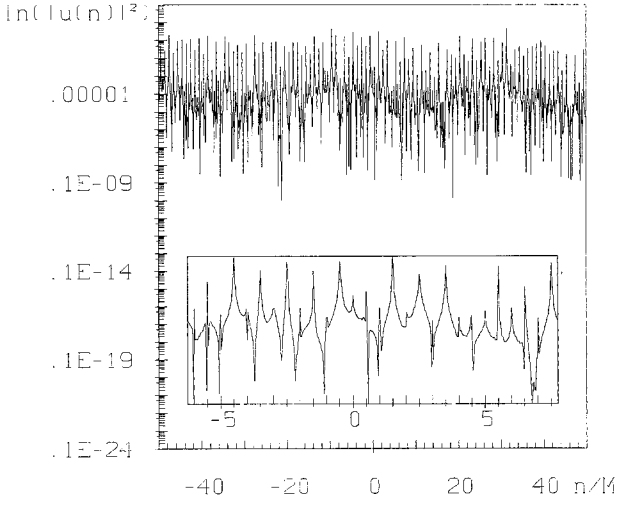

Fig. 2. The same as in Fig. 1 for $E=0.108$

3. Numerical solution

For the numerical solution of the Schrödinger equation we have employed 2 methods. In the first method we directly diagonalized the Hamiltonian in the $|n\rangle$ – basis restricted to $MN=7680$ states where M was taken up to 256, and N, the number of periodicity intervals, was taken up to 100. This method yields eigenstates and eigenvalues and is used to determine the eigenvalue statistics. Only the first case described at the end of Sect. 2 was treated by this method. As a second independent method we use the transfer matrix technique which yields Lyapunov exponents [7]. Here we have the possibility to make MN large, $MN=10^6$ in our calculations, and the largest M chosen was $M=256$. The localization length is always given in the number of periodicity intervals. We made special checks to confirm that M was sufficiently large so that this localization length did not depend on the size of M. The results are shown in Figs. 1–5.

In Fig. 1 we show one of the eigenstates determined by the first method using a basis of 3200 states for a periodicity interval of $m=32$ states, and $V=0.5$. The energy of this state is $E=0.471$ and therefore close to the middle of the gap $E=1/2$ of the system without randomness. The state is exponentially localized. A comparison with the localization length determined by the transfer matrix method is also given in the figure. The figure clearly shows the periodic peak structure with the period M, a part of which is shown on an amplified scale in the insert. As can be seen from this figure, a local periodic structure is preserved in the eigenstate, i.e. an approxi-

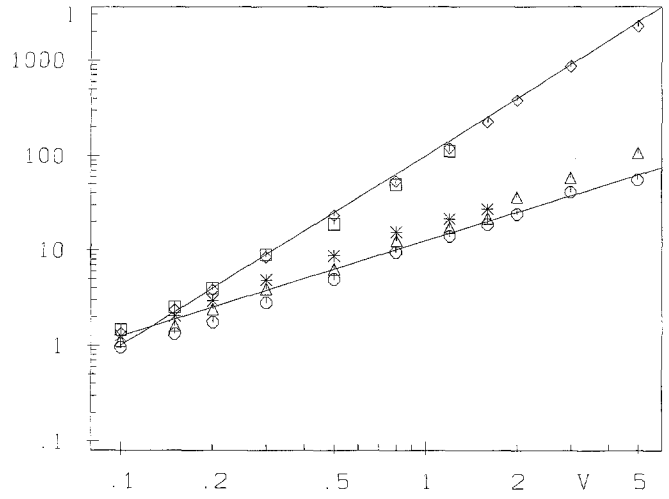

Fig. 3. Localization length l versus the matrix element $|V|$ in a doubly logarithmic plot. Different symbols correspond to case i) with quasi-energies in the band center (□), in the gap (○), in the middle between gap and band center (*), and case ii) (△). For comparison the data obtained in [6] for the matrix (2.4) in the band center are also shown (◇). The straight lines give l_A for the Anderson model in the band center and l_{DE}

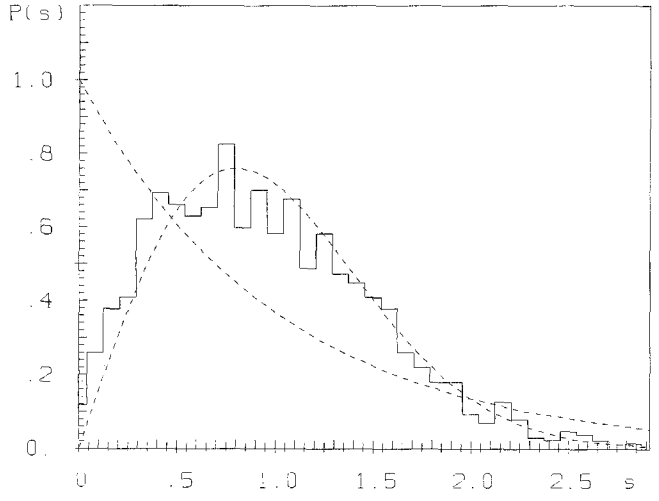

Fig. 4. Nearest neighbor level spacing distribution of the eigenstates for $V=0.5$, $M=256$, $N=6$. The dashed lines give the Poissonian and the Wigner distribution

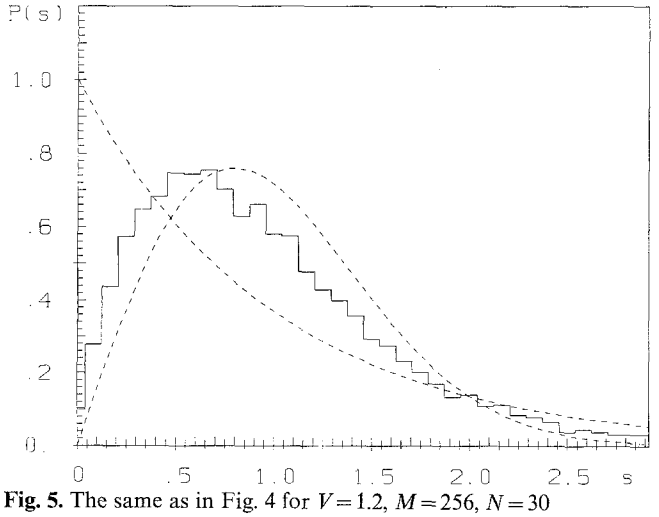

Fig. 5. The same as in Fig. 4 for $V=1.2$, $M=256$, $N=30$

mately conserved quasi-momentum quantum number should exist. In the closely related problem of periodically driven quantum system such a nearly conserved 'quasi-momentum' also appears. It has been introduced in the theory of periodically driven hydrogen atoms in [3].

In Fig. 2 another eigenstate with energy $E=0.108$ close to the band center at $E=0$ is shown. Otherwise all parameters are as in Fig. 1. This state has a much larger localization length which is no longer very small compared to the size of the finite basis. Again the periodic peak structure can be seen.

Next we turn to our results for the localization length l in the number of periodicity intervals obtained by the transfer matrix technique. In Fig. 3 we give in a doubly logarithmic plot l in the number of periodicity intervals as a function of the matrix element V. The upper curve was calculated for the case *i*) of Sect. 2 and gives l for states near the center of the band $E=0$. For comparison we also show the corresponding result for the band matrix of (2.4) which was obtained in a preceding paper [6]. The remarkable agreement shows that near the band center both models are nearly equivalent. The proportionality $l \simeq 90\,|V|^2$ at the band center and the coefficient agree well with the result $l_A \simeq 100\,|V|^2$ for the Anderson model at the band center [8]. The localization length for states away from the band center or in the gap are given in the lower curves in Fig. 3. Here we also give the result for case *ii*) of Sect. 2. In this case the localization length is independent of the energy. In the case *i*) in the middle of the gap $l \simeq 12\,|V|$, and in the middle between the band center and the gap $l \simeq 18\,|V|$. In the case *ii*) we find $l \simeq 18\,|V|$ independent of the energy. A linear dependence of l on $|V|$ for energies away from the band center was also found in [6] for the model described by the band matrix (2.4) and could there be understood by the similarity of the model with the Lloyd model [9]. In the present case the coefficients of proportionality are larger and do not agree as well with the Lloyd model, whose localization length is given, in the present notation, by $l_L = 2\pi\,|V|$ if $l_L \gg 1$. The physical mechanism for the $|V|$-proportionality is revealed by calculating the transition rate 2γ from a given state to a state in a neighboring periodicity interval. The golden rule gives

$$2\gamma = 2\pi\,|V|^2 \rho \tag{3.1}$$

but it is, of course, only valid for $|V|^2$ small. Following Deng and Eberly [10] we can extend the golden rule by including saturation effects. To this purpose we rewrite (3.1) as the ratio of the square of a Rabi frequency $|2V|$ and the total transition band width of the final state which is the sum of the 'static line width' $2/(\pi\rho)$ and the 'dynamic' width 2γ [10]

$$2\gamma = \frac{|2V|^2}{2(\pi\rho)^{-1} + 2\gamma} \tag{3.2}$$

For $\gamma \gg (\pi\rho)^{-1}$ one obtains the saturated transition rate $2\gamma = |2V|$, which equals the Rabi frequency of the transition. The localization length is proportional to 2γ and

hence to $|V|$, and the coefficient of proportionality can be obtained along the lines of Fishman et al. [11] as

$$l_{DE}=4\pi\gamma=4\pi|V| \tag{3.3}$$

The numerical results agree much better with (3.3) than with the Lloyd model result l_L, contrary to what was found in [6], where the numerical data were in better agreement with l_L. This might be connected with an important difference between the two models. While the present model describes the interaction between many sites, the one treated in [6] could be mapped on a model with nearest neighbor interaction only.

4. Level statistics

We can now use the numerical results to generate the nearest neighbor level spacing distribution (cf. [12]). An unfolding of the spectrum is not necessary as the model has a homogeneous averaged density of states. In Figs. 4, 5 we present our results for two different cases. Figure 4 was obtained for a basis of 1536 states, but the number of periodicity intervals contained in the basis was merely $N=6$. The matrix element was $V=0.5$, the same as in Figs. 1, 2. The localization length in this case changed between 5 and 20 and is not small compared to N. All localized states therefore overlap. For comparison the spacing distributions of the GOE statistics (full level repulsion) and the Poisson statistics (no level repulsion) are also given as dashed lines. It can be seen that the numerically determined levels show a slightly decreased level repulsion (the region $s\to 0$), but the overall agreement with the GOE statistics is rather good. We conclude that the periodic peak structure of the eigenstates does, in this case ($|V|=0.5$), not significantly influence the level spacing distribution. In Fig. 5 we choose $|V|=1.2$ and a basis size of 7680. The number of periodicity intervals included in this basis is $N=30$. Here the localization length changed between 14 and 100, i.e. l/N is still not small. Even though a significant distortion of the level spacing distribution compared to the GOE is noticeable, it is clearly not Poissonian. So it appears that the pronounced equidistant peak structure of the eigenstates has surprisingly little influence on the nearest neighbor level spacing distribution. A reason for this might be the fact that already a very small violation of a conservation law is sufficient to introduce level repulsion [12] and to destroy the Poissonian level spacing distribution.

5. Conclusions

We have presented a solid state model with a spatially modulated single-particle potential and a two-particle potential described by a band matrix. With randomness in the single-particle energies the model has localized states, which we determined numerically together with their localization length. The dependence of the localization length on the matrix element was determined under to different statistical assumptions on the single particle energies. The states were found to have a pronounced structure of peaks spaced at the periodicity interval. We have examined the nearest level spacing distribution of the energy levels and did not find a noticeable influence of the peak structure on the level repulsion.

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