Quantum Particle in One-Dimensional Potentials with Incommensurate Periods

M. Ya. Azbel
Bell Laboratories, Murray Hill, New Jersey 07974, and Department of Physics and Astronomy, Tel Aviv University, Ramat-Aviv, Tel-Aviv, Israel[a]

(Received 21 September 1979)

The energy spectrum and wave functions for a particle in periodic potentials with incommensurate periods are obtained analytically and reduced to specific phase trajectories. The spectrum is of the devil's-stairs type. States may be extended and localized, separated by mobility edges. These results are applicable to incommensurate linear chain structures (such as those in $Hg_{3-\delta}AsF_6$) and to the fine structure of de Haas–van Alphen oscillations.

The case of periodic potentials with incommensurate periods is interesting from several viewpoints: (a) It is a natural intermediate case between periodicity and randomness. (b) It allows for an explicity and physically vivid analytical solution[1-3] (see, e.g., some of the numerical solutions[4-6]). (c) It is related to electron properties of incommensurate linear structures [such as those[6-11] of $K_2Pt(CN)_4\cdot 3H_2O$, of tetrathiafulvalene-tetracyanoquinodimethane, of mercury chains[12] in $Hg_{3-\delta}AsF_6$], and to the fine structure[1,2] of de Haas–van Alphen and other quantum oscillations in high magnetic fields.

In this Letter, I prove that incommensurate potentials may provide extended states, and therefore metal conductivity; localized states, and therefore activation-type conductivity; non-Ohmic specific-resistivity dependence on the sample length; and metal-insulator transition.

First I elucidate the character of the spectrum and states; then relate them to specific phase trajectories; finally, I present the analytical solution and discuss its physical consequences.

I shall demonstrate the approach to the problem on the generalized Kronig-Penny model:

$$\psi''+(2m/\hbar^2)(E-U)\psi=0; \tag{1}$$

$$2mU/\hbar^2=\gamma\sum_{\Gamma=-\infty}^{\infty}\delta(x-x_r),\quad x_{r+1}-x_r=a_r, \tag{2}$$

with a_r being a periodic function of the (continuous) variable r,

$$a_r=f(\beta r),\quad f(\beta r+1)=f(\beta r)\geq 0, \tag{3}$$

with the (irrational) period $1/\beta$. We may assume $\beta<1$ [as the integer part of β is of no importance in Eq. (3) for integer r] and decompose it into a continued fraction,

$$\beta=1/(n_1+\beta_1)=1/[n_1+1/(n_2+\beta_2)]=\ldots, \tag{4}$$

where $0<\beta_1,\beta_2,\ldots<1$ and $n_1,n_2,\ldots$ are integers. The continuous fraction represents the process of measurement of the unit length segment with the β length segment. Suppose $1=\beta n_1+\beta\beta_1$ [and thus $\beta=1/(n_1+\beta_1)$], i.e., 1 contains n_1 segments β and a shorter segment whose length we denote as $\beta\beta_1<\beta$. Then we measure β with $\beta\beta_1$, which is equivalent to measuring 1 with β_1: $1=\beta_1 n_2+\beta_1\beta_2$, and so $\beta_1=1/(n_2+\beta_2)$, etc.

The decomposition (4) implied important physical consequences. Suppose $\gamma=\infty$ in Eq. (2). Then Eq. (1) provides a set of independent potential wells with spectra

$$E_r=\pi^2\hbar^2\mu_r^2/2ma_r^2,\quad \mu_r=1,2,\ldots, \tag{5}$$

which form the continuous spectrum. By Eqs. (3) and (5), the difference $\delta_j E_r\equiv E_{r+j}-E_r$ is determined mainly by the change δ_j in the fractional part of βj. For adjacent r's, $\delta_1=\beta$. When $j=n_1$ [n_1 is from Eq. (4)], then $\beta n_1=n_1/(n_1+\beta_1)=1-\beta_1/(n_1+\beta_1)=1-\beta\beta_1$, and thus $\delta_{n_1}=-\beta\beta_1$. Similarly, $\delta_{n_1n_2+1}=\beta\beta_1\beta_2$, etc. Thus when $\beta,\beta_1,\beta_2,\ldots\ll 1$, the adjacent wells provide n_1 levels with $\delta_1 E_r\propto\beta$; the wells separated by n_1 provide the splitting of each of these levels into n_2 sublevels, separated by $\delta_{n_1}E_r\propto\beta\beta_1$; each of the sublevels is split into subsublevels with $\delta_{n_1n_2}E_r\propto\beta\beta_1\beta_2$, etc. Thus, there appear the devil's stairs of the levels, related to the decomposition (4). The spectrum has a singular point at each rational β, when the number of stairs becomes finite [then finite γ in Eq. (2) widens the last stair levels into narrow bands of the corresponding periodic potential].

Now suppose γ in Eq. (2) is finite (and, e.g., positive). The rth well (with $x_r\leq x\leq x_{r+1}$) provides

$$\psi=A_r'\exp[i\kappa(x-x_r)]+A_r\exp[-i\kappa(x-x_r)], \tag{6}$$
$$\kappa=(2mE/\hbar^2)^{1/2}.$$

Matching ψ and $d\psi/dx$ at the boundary $x=x_{r+1}$ between the rth and the $(r+1)$st wells, we obtain the recurrence relations for A_r and A_r'. De-

coupling them and using the displacement operator $\exp(\beta d/d\xi)$, we obtain the infinite-order differential equation for A_r:

$$\hat{H}A(\xi)=0, \quad A(\xi)\equiv A(\beta r)\equiv A_r, \tag{7}$$

$$\hat{H}=\tfrac{1}{2}[\exp(2\pi i\hat{p})+\exp(i\theta)\exp(-2\pi i\hat{p})\exp(-i\theta)] - (\cos\theta+\epsilon\sin\theta), \tag{8}$$

$$\theta(\xi)=\theta(\xi+1)=\kappa f(\xi),$$

$$\hat{p}=(\beta/2\pi i)d/d\xi, \epsilon=\tfrac{1}{2}\gamma/\kappa. \tag{9}$$

Equation (9) is the "Schrödinger equation"[13] in the "momentum p"-"coordinate ξ" space, with β being the "Planck constant". The nature of the solution is determined by "classical" (with respect to β) "phase trajectories" (later denoted as PT), which correspond to $\hat{p}$ replaced by a number p,

$$\cos(2\pi p)=\sin(\theta+\Lambda)/\sin\Lambda, \quad \Lambda=\operatorname{arccot}\epsilon. \tag{10}$$

The character of these PT is demonstrated in Fig. 1. They start with localized states of closed PT (of the α_1 type), which are separated by the mobility edge (PT α_2) from the states extended in ξ of open PT (of the α_3 type) separated by another mobility edge (PT α_4) from other localized states (of the α_5, α_6 type), some of which (of the α_6 type) are separated by the mobility edge (PT α_7) from the states (of the α_9 type) extended in p, etc. Each PT is explicitly related by Eqs. (9) and (10) to $f(\xi)$, κ, and γ, of the initial Hamiltonian of Eq. (1).

The next (quasiclassical) approximation provides the Bohr quantization[1,2,14-16]

$$S=(q+\tfrac{1}{2}+\eta)\beta, \tag{11a}$$

where S is the area of PT, β stands for the "Planck constant"; q is integer and $|\eta|<\frac{1}{2}$ (for closed PT, remote from the mobility edge, $\eta\simeq 0$). Quasiclassical wave functions oscillate in the classically available region, and exponentially (with $-1/\beta$) decay outside of this region.[14-16]

The next approximation accounts for the interaction of PT due to the "particle" tunneling between them (e.g., from α_5' to α_5'' in Fig. 1), similarly to the well-known magnetic breakdown.[16] A "particle", described by Eq. (7), can drift through the whole (p,ξ) plane, as p and ξ enter $\hat{H}$ in a symmetric way. More specifically, $\hat{H}$ commutes with unitary "periodic coordinate" and "periodic momentum" operators $\hat{Q}=\exp(2\pi i\xi/\beta)$ and $\hat{P}=\exp(2\pi i\hat{p}/\beta)\equiv\exp(d/d\xi)$. (If $\beta=r/s$ with integer r and s, then $\hat{Q}^r$ and $\hat{p}$ commute themselves.) Thus, the Bloch theorem is valid

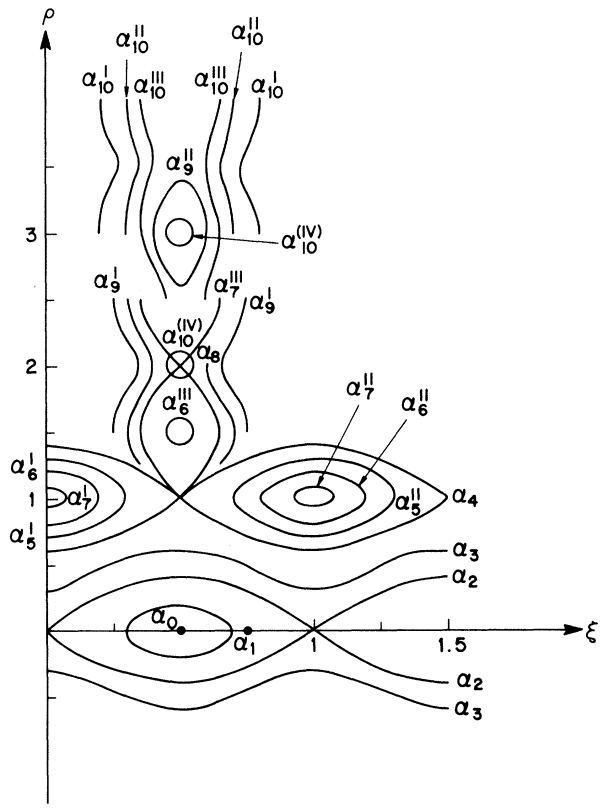

FIG. 1. Characteristic phase trajectories (PT) of Eq. (11). The values of κ_k for PT α_k are related to $\tilde{\theta}_k=\kappa_k\min[f(\xi)]\equiv\kappa_k\tilde{a}$; $\theta_k=\kappa_k\max[f(\xi)]\equiv\kappa_k a$; $\Lambda_k=\arctan(2\kappa_k/\lambda)$ by the equations $\theta_0=\pi-2\Lambda_0$ (the spectrum starting point); $\tilde{\theta}_1<\pi-2\Lambda_1<\theta_1<\pi$; $\tilde{\theta}_2=\pi-2\Lambda_2<\theta_2<\pi$; $\pi-2\Lambda_3<\tilde{\theta}_3$, $\theta_3<\pi$; $\pi-2\Lambda_4<\tilde{\theta}_4$, $\theta_4=\pi$; $\pi-2\Lambda_5<\tilde{\theta}_5<\pi<\theta_5<2\pi-2\Lambda_5$; $\pi-2\Lambda_6<\tilde{\theta}_6<\pi$, $2\pi-2\Lambda_6<\theta_6<2\pi$; $\pi-2\Lambda_7<\tilde{\theta}_7<\pi$, $\theta_7=2\pi$; $\pi<\tilde{\theta}_8<2\pi-2\Lambda_8$, $2\pi<\theta_8<3\pi-2\Lambda_8$; $\pi<\tilde{\theta}_9<2\pi-2\Lambda_9$, $3\pi-2\Lambda_9<\theta_9<3\pi$; $2\pi-2\Lambda_{10}<\tilde{\theta}_{10}<2\pi$, $5\pi-2\Lambda_{10}<\theta_{10}<5\pi$. In the case of $\gamma a\ll 1$ and $\tilde{a}<\frac{1}{2}a$, the spectrum starts with $\kappa_0=\sqrt{\gamma}/a$, and the mobility edges have $\kappa_2=\sqrt{\gamma}/\tilde{a}$; $\kappa_4=\pi/a$; $\kappa_7=2\pi/a$. The picture is periodic with p and ξ. Different PT with the same κ are denoted by superscripts.

for A both in coordinate and momentum representations. This implies a very specific character of the energy spectrum and wave functions.

Because of the periodicity of $H(p,\xi)$, Eq. (7) is an infinite-order differential equation. Its general solution can be presented in the following form[3]:

$$A(\xi)=A_1^{(1)}(\xi)\alpha^{(1)}(\xi)+A_1(\xi)\alpha^{(2)}(\xi)\equiv\vec{A}_1\cdot\vec{\alpha}, \tag{11}$$

where $\alpha^{(1)}$ and $\alpha^{(2)}$ are any two independent solutions of Eq. (7) (e.g., the quasiclassical ones), and $A_1^{(1)}$, A_1 are arbitrary periodic functions with the period β [which replace the arbitrary

constants of a finite-order differential equation [cf. Eq. (6)].

As $\vec{\alpha}(\xi+1)=\hat{P}\vec{\alpha}(\xi)$ is also the solution of Eq. (7), and so, by Eq. (11),

$$\vec{\alpha}(\xi+1)=\hat{g}(\xi)\vec{\alpha}(\xi),\quad \hat{g}(\xi+\beta)=\hat{g}(\xi). \tag{12}$$

Bloch's theorem, applied to $A(\xi)$, by virtue of Eqs. (4), (11), and (12), provides the equation for A_1, which can be reduced to the same type of equation as Eq. (7), but with β_1, A_1, replacing β, A. So, the "magnetic breakdown" between PT implies the dependence of $\vec{A}_1$ in Eq. (11) on ξ and relates this dependence to a new set of PT with the corresponding spectrum and wave functions. The magnetic breakdown between these new PT, in its turn, leads to the next stair in the devil's stairs, and so on.

Thus, the $\psi(x)$ from Eq. (6) for an arbitrary r and $x-x_r$ is related to $A_r\equiv A(\beta r)$, and therefore, on account of Bloch's theorem, to $A(\beta r-[\beta r])$ (where square brackets denote the integer part), and thus, by Eqs. (4) and (11), to $\vec{A}_1(\beta r-[\beta r])=\vec{A}_1(-[\beta r])=\vec{A}_1(-\beta[\beta r]/\beta)=\vec{A}_1(-\beta\beta_1[\beta r])$ (as $1/\beta=n_1+\beta_1$ and A_1 has a period β), and so on. Each of these "wave functions" has its own classical PT and quasiclassics. For instance, quasiclassical $\vec{\alpha}(\beta r)$ is related to the period 1, and thus essentially changes when r changes by $\delta r\sim 1/\beta$ and x [according to Eq. (2)] by $\delta x\sim a/\beta$. At this distance, $q(x)=|\psi(x)|^2$ oscillates in classically available region and exponentially decays outside it. Quasiclassical $\vec{A}_1(-\beta\beta_1[\beta r])$ is related to its period β, and thus essentially changes at $\delta r\sim 1/\beta\beta_1$ and $\delta x\sim a/\beta\beta_1$, providing the modulation of $q(x)$, related to $\delta x\sim a/\beta\beta_1$ and to PT of the next stair.

The crucial differences in the Hamiltonian are those which provide the change in the topology of PT. For instance, a "tight-binding" equation,

$$\tfrac{1}{2}(\psi_{r+1}+\psi_{r-1})+\cos(2\pi\beta r)\cdot\psi_r=\lambda\psi_r, \tag{13}$$

has only two types of closed PT with the mobility-edge–type PT between them. It is convenient to demonstrate the analytical formulas with this simple example. Here the equations for the next-stair functions are universal and coincide with Eq. (13) with β and λ replaced by β_1, λ_1, etc. The spectrum of Eq. (13) is described[3] by Eq. (11a), where

$$\eta=2[\sigma(\ln\sigma-1)-\operatorname{Im}\ln\Gamma(\tfrac{1}{2}+i\sigma)]-(-1)^q\arcsin[2\lambda_1/\cosh(\pi\sigma)], \tag{14}$$

$$\sigma=|\lambda|/\beta; \tag{15}$$

Γ is the Γ function. When $\sigma\gg 1$, then $\eta\propto\exp(-\pi\sigma)$.

Equation (13) also describes[1,2] a magnetic breakdown in a high magnetic field, parallel to a crystal symmetry axis. The devil's-stairs–type spectrum implies then the fine structure of de Haas–van Alphen oscillations.[2]

The electronic density $\rho(x)$ (described above) determines the resistivity R. Just as in the case of a random potential,[17,18] localized states provide the activation resistivity, while extended states imply the metallictype resistivity (this may be the case[12] in $Hg_{3-\delta}AsF_6$). But even in the latter case, an infinite scale of lengths a/β, $a/\beta\beta_1,\ldots$ (which is similar to the situation in a random case) will allow for the Ohm's law $R\propto L$ (L is the sample length) only with the accuracy of the devil's stair, related to $L\sim a/\beta_1\beta_2\ldots\beta_K$; the higher accuracy implies oscillatory dependence on L.

The change in, e.g., the external pressure, may change the character (localized or extended) of the Fermi-energy state and thus provide a metal-insulator transition.

This Letter was initiated while the author was working at Brookhaven National Laboratory. This research was thus supported in part by the Division of Basic Energy Science, U. S. Department of Energy, under Contract No. EY-76-C-02-0016.

I am very grateful to Professor P. W. Anderson for a helpful discussion. The discussions following talks at Brookhaven National Laboratory and Bell Laboratories are also highly appreciated.

---

[a]Permanent address.

[1]M. Ya. Azbel, Zh. Eksp. Teor. Fiz. 44, 980 (1963) [Sov. Phys. JETP 17, 665 (1963)].

[2]M. Ya. Azbel, Zh. Eksp. Teor. Fiz. 46, 929 (1964) [Sov. Phys. JETP 19, 634 (1964)].

[3]M. Ya. Azbel, Dokl. Akad. Nauk SSSR 159, 703 (1964) [Sov. Math. Dokl. 5, 1549 (1964)].

[4]S. Aubry, in *Solid State Sciences: Solitons and Condensed Matter Physics*, edited by A. P. Bishop and T. Schneider (Springer, Berlin, 1978), Vol. 8, p.264.

[5]S. Aubry and G. Andre, in Colloquium on Group Theoretical Methods in Physics, Kiryat Anavim, Israel, 1979 (to be published).

[6]R. A. Guyer and M. D. Miller, Phys. Rev. Lett. 42, 718 (1979).

[7]P. Bruesch, S. Strassler, and H. R. Zeller, Phys. Rev. B 12, 219 (1975).

[8]L. B. Coleman, M. J. Cohen, D. J. Sandman, F. G. Yagamishi, A. F. Garito, and A. J. Heeger, Solid State Commun. 12, 1125 (1973).

[9]M. J. Rice, A. R. Bishop, J. A. Krumhansl, and S. E. Trullinger, Phys. Rev. Lett. 36, 432 (1976).
[10]M. J. Cohen, P. R. Newman, and A. J. Heeger, Phys. Rev. Lett. 37, 1500 (1976).
[11]R. A. Guyer and M. D. Miller, Phys. Rev. A 17, 1174 (1978).
[12]C. K. Chiang, R. Spal, A. Denenstein, A. J. Heeger, N. D. Miro, and A. G. MacDiarmid, Solid State Commun. 22, 293 (1977).
[13]Equation (8) can be transformed into the Hermitian form.
[14]G. E. Zilberman, Zh. Eksp. Teor. Fiz. 32, 296, and 33, 387 (1957), and 34, 748 (1958).
[15]M. Ya. Azbel, Zh. Eksp. Teor. Fiz. 39, 1276 (1960).
[16]I. M. Lifshitz, M. Ya. Azbel, and M. I. Kaganov, *Electron Theory of Metals* (Consultant Bureau, New York, 1973).
[17]N. F. Mott and W. D. Twose, Adv. Phys. 10, 107 (1961).
[18]D. J. Thouless, Phys. Rep. 13C, 94 (1974).

New Model Hamiltonian for the Metal-Insulator Transition

C. Castellani
Istituto di Fisica, Università dell'Aquila, Aquila, Italy, and Istituto di Fisica "G. Marconi," Università di Roma, Roma, Italy, and Gruppo Nazionale di Struttura della Materia del Consiglio Nazionale delle Ricerche, Sezione dell'Aquila, Italy

and

C. Di Castro
Istituto di Fisica "G. Marconi," Università di Roma, Roma, Italy, and Gruppo Nazionale di Struttura della Materia del Consiglio Nazionale delle Ricerche, Sezione di Roma, Italy

and

D. Feinberg and J. Ranninger
Groupe des Transitions de Phases, Centre National de la Recherche Scientifique, Laboratoire Associée à l'Université Scientifique et Médicale de Grenoble, Grenoble, France

(Received 28 June 1979)

With use of the symmetry properties of the half-filled single-band Hubbard Hamiltonian, there is derived an effective Hamiltonian on a decimated lattice in which the spin and charge operators occur explicitly. Being a generalization of the Blume-Emery-Griffiths Hamiltonian for He^3-He^4 mixtures, this new statistical mechanical model permits one to give a preliminary discussion of the phase diagram of the correlated electron gas by establishing analogies with their results.

It is generally accepted that the metal-insulator transition, when described exclusively on the basis of electron correlation on a lattice with one electron per site, is due to a competition between the delocalizing effect of the hopping term and the localizing effect of the on-site repulsive Coulomb interaction as described by the Hubbard Hamiltonian[1]:

$$H = \sum_{i,j}\sum_{\sigma} t_{ij}\, c_{i\sigma}{}^{\dagger} c_{j\sigma} + U\sum_i n_{i\uparrow} n_{i\downarrow}. \qquad (1)$$

Here $c_{i\sigma}{}^{\dagger}$ and $c_{i\sigma}$ are the creation and annihilation operators of an electron with spin σ in a Wannier state $\varphi_i(\vec{x})$ at site i and $n_{i\sigma}=c_{i\sigma}{}^{\dagger}c_{i\sigma}$ are the corresponding occupation numbers. We suppose that the hopping integrals $t_{ij}=t$ are nonzero only for nearest-neighbor sites.

It is still an open question whether this model is really capable of reproducing the anticipated phase diagram,[2,3] which is expected to show at least the following three features with the variation of the temperature: (1) a second-order phase transition from a paramagnetic insulator to an antiferromagnetic insulator when U is large in comparison with the bandwidth $W=2zt$ (z is the number of nearest neighbors in a simple cubic lattice); (2) a first-order phase transition from an antiferromagnetic insulator to a metal when U is small in comparison with W; (3) a first-order phase transition from a metal to a paramagnetic insulator when U is comparable with W.

So far nothing conclusive has been stated in the literature concerning the number and the nature of the intersection points of the various coexistence curves. In fact, only the first feature has been unquestionably established since for $U \gg W$, the Hubbard Hamiltonian becomes equivalent to the Heisenberg Hamiltonian.[2] The relevant quantities in this case are the local spin operators, each site being occupied by one electron with either spin up or spin down.

