Transport properties of an incommensurate system

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The exactly solvable model of Grempel, Fishman, and Prange of a particle in a potential having two periods is discussed. If the ratio of the periods is a typical irrational the states are all localized. A convenient form for the Green's function of the model is given and used to obtain a simple expression for the ac conductivity. In the one-dimensional case, the frequency and temperature dependence of the conductivity is found and the crossover to Mott phonon-assisted hopping is discussed. An expression for the transmission coefficient is found and its length dependence and resonances are considered.

I. INTRODUCTION

Recently Grempel, Fishman, and Prange in a series of papers[1-3] have discussed an interesting, exactly solvable model of quantum motion in an incommensurate potential. In one form the model is a tight-binding model

$$(t_n-\varepsilon)a_n+W(a_{n-1}+a_{n+1})=0\ , \tag{1.1}$$

where a_n is the amplitude of the wave function on site n, W is the nearest-neighbor hopping matrix element, ε is the energy, and $t_n=\tan[(\alpha-n\tau)/2]$, where α is a phase and $\tau/2\pi$ can be rational or irrational. The model (1.1) was solved by Grempel *et al.*[1] by noting that it is equivalent to a kicked oscillator and they showed that the model (for most irrational τ) has only localized eigenstates (in all dimensions[3]). This is a result of the special form of the site energies t_n. The model is related to the Lloyd model[4] for disorder—the distribution of site energies for most irrational τ is a Cauchy distribution and the localization length and average density of states are the same as the Lloyd model.

Further insight into this model can be obtained by considering its dual. Assume $\tau=2\pi p/N$, where p and N are coprime and are the convergents of the irrational $\tau/2\pi$ of interest. The irrational case is then obtained in the limit $p, N\to\infty$. To obtain the dual of (1.1) we introduce

$$a_n=\frac{1}{\sqrt{N}}\sum_{m=0}^{N-1}e^{inm\tau}\hat{a}_m \tag{1.2}$$

and on substituting in (1.1) we find the equation for the $\hat{a}_m$

$$[2W\cos(m\tau)-\varepsilon]\hat{a}_m+\sum_r U_r\hat{a}_{m+r}=0\ , \tag{1.3}$$

where

$$U_r=\frac{1}{N}\sum_{n=0}^{N-1}e^{inr\tau}\tan\left[\frac{\alpha-n\tau}{2}\right]\ . \tag{1.4}$$

Using the (nonconvergent) Fourier expansion

$$\tan x=2\sin 2x-2\sin 4x\ldots$$

we find

$$U_r=-i(e^{i\alpha}\delta_{r,1}-e^{-i\alpha}\delta_{r,-1})+i(e^{2i\alpha}\delta_{r,2}-e^{-2i\alpha}\delta_{r,-2})+\cdots\ . \tag{1.5}$$

Then the dual of (1.1) involves long-range hopping and we would expect the dual states to be extended.

This model provides an interesting case in which the transport properties of a system possessing localized states can be discussed in some detail. In Sec. II we give the solution of the tight-binding model (1.1) and discuss some properties of the solution. This section is mainly given for completeness and follows the work of Grempel *et al.*[1] quite closely. In Sec. III we discuss the Green's function for this model. The Green's function has also been obtained by Pastur and Figotin[5] by a different method. In Sec. IV we use the Green's function to obtain a simple expression for the ac conductivity and discuss its frequency and temperature dependence. The low-frequency conductivity at zero temperature has been discussed by Prange *et al.*[6] and Pastur and Figotin[5] and our results are in agreement with theirs. In Sec. V we discuss Mott hopping conductivity for this incommensurate, localized model. In Sec. VI we derive an expression for the transmission coefficient of a finite length of the incommensurate system and discuss the conductivity, its length dependence and its resonances. Most of our results in this paper are for the one-dimensional case but the model (1.1) is solvable in all dimensions[3] and number of our results can be extended to higher dimensions.

II. TIGHT-BINDING MODEL

The model (1.1) was solved by Grempel *et al.*[1] by noting that it is equivalent to a periodically kicked oscillator. For our purposes it is simpler to solve the model directly,

although the procedure is not very different. As noted above we take $\tau=2\pi p/N$, where p and N are the convergents of the irrational number $\tau/2\pi$ of interest. The potential then has period N and the irrational case is obtained as the limit $p,N\to\infty$. We first investigate solutions in which $a_{n+N}=a_n$. These provide a complete set. Introducing the Fourier transform

$$a_n=\frac{1}{\sqrt{N}}\sum_k e^{ikn}u_k \ , \tag{2.1}$$

where $k=2\pi l/N$ ($l=1\ldots N$) in (1.1) we obtain

$$\sum_k e^{ikn}u_k(t_n-\varepsilon+2W\cos k)=0 \ . \tag{2.2}$$

Following Grempel *et al.* let $\varepsilon-2W\cos k=\tan V(k)/2$ and this equation can be written as

$$\sum_k e^{ikn}\bar{u}_k(e^{-(i/2)V(k)}-e^{-i[\alpha-n\tau-V(k)/2]})=0 \ , \tag{2.3}$$

where $u_k=\bar{u}_k\cos V(k)/2$. As τ is of the same form as k, we can set $k+\tau=k'$ in the second term of (2.3) and obtain the relation

$$\bar{u}_{k+\tau}=\bar{u}_k e^{-(i/2)[2\alpha-V(k+\tau)-V(k)]} \ . \tag{2.4}$$

Using the conditions $\bar{u}_{k+2\pi}=\bar{u}_k$, $\bar{u}_{-k}=\bar{u}_k^*$ we set

$$\bar{u}_k=e^{-i\nu k+i\phi(k)} \ , \tag{2.5}$$

where ν is an integer and $\phi(-k)=-\phi(k)$. From (2.4) we find

$$\phi(k+\tau)-\phi(k)=\nu\tau-\alpha+\tfrac{1}{2}[V(k+\tau)+V(k)]-2\pi l \ , \tag{2.6}$$

where l is an integer. Introducing the Fourier series

$$V(k)=\sum_{n=0}^{N-1}V_n e^{ikn} \ , \qquad \phi(k)=\sum_{n=1}^{N-1}\phi_n e^{ikn} \ , \tag{2.7}$$

in (2.6) we find

$$\alpha-\nu\tau+2\pi l=V_0(\varepsilon) \ , \tag{2.8}$$

$$\phi_n=-(i/2)\cot(n\tau/2)V_n \ , \tag{2.9}$$

where Eq. (2.8) is the eigenvalue condition. For later purposes it is convenient to introduce

$$\theta(k)=\tfrac{1}{2}\sum_{n=1}^{N-1}V_n\frac{\sin(nk)}{\sin(n\tau/2)} \ . \tag{2.10}$$

From (2.5) and (2.7) the (unnormalized) wave function can then be written as

$$a_n^{(\nu)}=\cos\left[\frac{n\tau-\alpha}{2}\right]F_{n-\nu} \ , \qquad F_n=\frac{1}{N}\sum_k e^{ikn+i\theta(k)} \ . \tag{2.11}$$

These eigenstates can be shown to be orthogonal. In one dimension we note that

$$V_n=V_{N-n}=-\frac{2}{n}e^{-\gamma n}\sin(\mu n) \ , \tag{2.12}$$

where

$$\cosh(\gamma)\cos\mu=\varepsilon/2W, \quad \sinh(\gamma)\sin\mu=1/2W \ . \tag{2.13}$$

The eigenstates have been discussed in detail by Prange, Grempel, and Fishman.[2] For most irrationals they are exponentially localized with a localization length γ^{-1}. This is the case of interest in this paper. The integer ν can be regarded as the band index for N finite or as the center of the localized state in the limit $N\to\infty$. From (2.8) it follows that the average density of states is

$$\rho(\varepsilon)=\frac{1}{2\pi}\frac{\partial V_0}{\partial\varepsilon} \ .$$

This can be shown to be identical with that in the Lloyd model.

More general solutions of (1.1) can be obtained as follows. The potential t_n has period N and thus the unit cell has N sites and we expect N bands of states. From the Bloch theorem we can write $a_n=e^{iqn}a_{q,n}$, where $a_{q,n+N}=a_{q,n}$ has the period of the unit cell and the wave vector q $[-(\pi/N)<q<(\pi/N)]$ labels the states within each of the N bands. Proceeding as above the eigenvalue condition replacing (2.8) is

$$\alpha-\nu\tau-2\pi l=\frac{2}{N}\sum_k\tan^{-1}[\varepsilon-2W\cos(k+q)] \ . \tag{2.14}$$

As the band index ν varies from 1 to N, $\nu\tau$ (mod2π) takes on the values $(2\pi/N)l$ ($l=1\ldots N$) but not in this order. Thus $\nu\tau$ for two neighboring energy bands (in energy) will differ by $2\pi/N$ (mod2π) and thus from (2.10) the energy bands are separated in energy by $1/\rho N$. For a given band the wave vector q lies between $\pm\pi/N$ and thus the energy width of a band is of order $1/N^2$. In the limit $N\to\infty$ for typical irrationals we get a discrete spectrum of localized states. A much more detailed discussion of the eigenstates is given in Ref. 2.

For a discussion of transport properties it is useful to know how the states are distributed in space and in energy. The eigenvalue of the state localized at site ν is determined by (2.8) and we discuss the formula in the case where $\tau/2\pi$ approaches the golden mean. Then τ is approximated by $\tau=2\pi f_k/f_{k+1}$, where the f are Fibonacci numbers ($f_0=f_1=1$) and the unit cell is of length f_{k+1}. Suppose we have a localized state ν centered at site ν and consider the state $\nu\pm f_p$ which is localized f_p steps away. The difference in energy of these two states is given by

$$V_0(\varepsilon_{\nu\pm f_p})-V_0(\varepsilon_\nu)=\mp f_p\tau \ (\text{mod}2\pi)$$

$$=\mp(-1)^p 2\pi\frac{f_{k-p}}{f_{k+1}} \ (\text{mod}2\pi) \ , \tag{2.15}$$

where we have used the relation $f_k f_p=f_{k+1}f_{p-1}+(-1)^p f_{k-p}$. If $p<k$ we can expand (2.15) and find

$$\varepsilon_{\nu\pm f_p}-\varepsilon_\nu=\mp(-1)^p f_{k-p}/\rho f_{k+1} \ , \tag{2.16}$$

where ρ is the density of states. For large k and p, $f_p \sim \phi^{p+1}/\sqrt{5}$ where $\phi = \frac{1}{2}(1+\sqrt{5})$ and

$$\varepsilon_{\nu \pm f_p} - \varepsilon_\nu = \mp \frac{(-1)^p}{\rho \phi^{p+1}} = \mp \frac{(-1)^p}{\rho \sqrt{5} f_p} . \tag{2.17}$$

We note the following special cases:

(i) $p=0$ $|\varepsilon_{\nu+1} - \varepsilon_\nu| \sim \tau/2\pi\rho$ so that states which are nearest neighbors in space have a large energy separation.

(ii) $p=k$ $|\varepsilon_{\nu \pm f_k} - \varepsilon_\nu| \sim 1/\rho\sqrt{5} f_k$ so that eigenstates which are near neighbors in energy have a large spatial separation.

These results will be useful in the discussion of hopping conductivity. They are special to the case where $\tau/2\pi$ approaches the golden mean but similar results should apply to other quadratic or common irrationals. Equation (2.17) does not take into account all the energy levels because the f_p do not cover all the integers but does include the levels closest in energy to a given level which are of most interest to us.

III. THE GREEN'S FUNCTION

The Green's function is the solution of

$$(t_m - \varepsilon) G_{mn} + W(G_{m+1,n} + G_{m-1,n}) = \delta_{m,n} \tag{3.1}$$

and this can be solved in a similar manner to that used in Sec. II. G_{mn} does not depend on $m-n$ but we can take the Fourier transform on m and write

$$G_{mn} = \frac{1}{N} \sum_k e^{ik(m-n)} G(k) , \tag{3.2}$$

where $G(k)$ still depends on n. Substituting in (3.1) and following the same steps that led to (2.3) we obtain

$$\sum_k e^{ik(m-n)} [\bar{G}_k e^{-iV_k/2} - \bar{G}_k e^{-i(\alpha - m\tau - V_k/2)} - i(1 + e^{-i(\alpha - n\tau)})] = 0 , \tag{3.3}$$

where $G_k = \cos[V(k)/2]\bar{G}_k$. Shifting k to $k-\tau$ in the second term and equating the coefficient of e^{ikm} to zero gives

$$\bar{G}_k e^{-iV_k/2} - \bar{G}_{k-\tau} e^{-i(\alpha - n\tau - V_{k-\tau}/2)} = i(1 + e^{-i(\alpha - n\tau)}) . \tag{3.4}$$

We put $\bar{G}_k = A(k) e^{i\phi(k)}$, where $\phi(k)$ is given by (2.7) and (2.9) and use the relations

$$\begin{aligned} \phi(k) - \tfrac{1}{2} V(k) &= \theta(k - \tau/2) - \tfrac{1}{2} V_0 , \\ \phi(k-\tau) + \tfrac{1}{2} V(k-\tau) &= \theta(k - \tau/2) + \tfrac{1}{2} V_0 . \end{aligned} \tag{3.5}$$

Then

$$A(k) - A(k-\tau) e^{-i(\alpha - n\tau - V_0)} = i e^{-i[\theta(k - \tau/2) - V_0/2]} (1 + e^{-i(\alpha - n\tau)}) . \tag{3.6}$$

This can be solved by expanding $A(k)$ in a Fourier series

$$A(k) = \sum_{n'=0}^{N-1} e^{ikn'} A_{n'}$$

and it is found that

$$A_{n'} = \frac{c_n}{\sin\{\frac{1}{2}[\alpha - V_0 + (n'-n)\tau]\}} F_{n'} , \tag{3.7}$$

where F_n is given in (2.11) and $c_n = \cos[\frac{1}{2}(\alpha - n\tau)]$. After some straightforward algebra we find

$$G_{mn} = \sum_{n'} \frac{c_n \cos\{\frac{1}{2}[V_0 - \tau(m-n')]\}}{\sin[\frac{1}{2}(\alpha - V_0 - n'\tau)]} F_{n-n'} F_{m-n'} . \tag{3.8}$$

This can also be written in the symmetric form

$$G_{mn} = c_m c_n \sum_{n'} \cot[\tfrac{1}{2}(\alpha - V_0 - n'\tau)] F_{m-n'} F_{n-n'} + \tfrac{1}{2} \sin(\alpha - m\tau) \delta_{m,n} . \tag{3.9}$$

The Green's function depends on ε most importantly through the $V_0(\varepsilon)$ under the cotangent. The functions F are weakly dependent on ε. The $F_n \sim e^{-\gamma|n|}$ for large n and thus the Green's function is short ranged and proportional to $e^{-\gamma|m-n|}$ for large $|m-n|$. Replacing $\varepsilon \to \varepsilon + i\eta$, where η is small and positive we find

$$\mathrm{Im} G_{mn} = \pi c_m c_n \sum_{n'} \delta(\sin\tfrac{1}{2}(\alpha - V_0 - n'\tau)) F_{m-n'} F_{n-n'} , \tag{3.10}$$

which will be useful in calculating the conductivity in Sec. IV. The average density of states can also be obtained by averaging $\mathrm{Im} G_{mm}$ over sites m. A different form of the Green's function has been given by Pastur and Figotin.[5]

IV. ac CONDUCTIVITY

The Kubo formula for the ac conductivity at frequency ω when expressed in terms of the imaginary part of the Green's function is

$$\sigma(\omega) = \frac{e^2 W^2}{\omega N \pi} \int d\varepsilon [f(\varepsilon') - f(\varepsilon)] \sum_{n,m} \{[\mathrm{Im} G_{n+1,m}(\varepsilon) \mathrm{Im} G_{m+1,n}(\varepsilon') - \mathrm{Im} G_{n+1,m+1}(\varepsilon) \mathrm{Im} G_{m,n}(\varepsilon')] + (\varepsilon \leftrightarrow \varepsilon')\} , \tag{4.1}$$

where $\varepsilon' = \varepsilon - \omega$ and f is the Fermi function. Substituting from (3.10) for the Green's function, averaging over the phase α, and taking the limit as $N \to \infty$ gives

$$\bar{\sigma}(\omega) = \frac{e^2 W^2}{\omega} \int d\varepsilon [f(\varepsilon') - f(\varepsilon)] \sum_{n=-\infty}^{\infty} \delta(\sin\{\tfrac{1}{2}[V_0(\varepsilon) - V_0(\varepsilon') - n\tau]\}) H_n^2 , \tag{4.2}$$

where

$$H_n=\sum_m[\bar{F}_{m+1}(\varepsilon)\bar{F}_{m-n}(\varepsilon')-\bar{F}_m(\varepsilon)\bar{F}_{m+1-n}(\varepsilon')] \tag{4.3}$$

and

$$\bar{F}_m(\varepsilon)=\cos\{\tfrac{1}{2}[V_0(\varepsilon)-m\tau]\}F_m(\varepsilon)\ .$$

Using the results (2.7), (2.10), and (3.5) it is not difficult to show that

$$H_n=\frac{2i}{N}\sum_k e^{ikn}\sin(k)\cos\left[\frac{V(k)}{2}\right]\times\cos\left[\frac{V'(k)}{2}\right]e^{i[\phi(k)-\phi'(k)]}\ , \tag{4.4}$$

where $V(k)=V(k,\varepsilon)$, $V'(k)=V(k,\varepsilon')$, and similarly for $\phi(k)$ and $\phi'(k)$. This expression does not depend sensitively on $\omega=\varepsilon-\varepsilon'$ and at low frequencies setting $\varepsilon=\varepsilon'$ in (4.4) we obtain (for $N\to\infty$)

$$H_n=\frac{i}{\pi}\int_\pi^\pi dk\, e^{ikn}\sin(k)\cos^2\left[\frac{V(k)}{2}\right]$$

$$=\frac{4}{W}e^{-\gamma|n|}\sin(\mu n)+\tfrac{1}{2}(\delta_{n-1,0}-\delta_{n+1,0})\ . \tag{4.5}$$

At low frequencies the terms with $n=\pm1$ do not contribute to (4.2) and substituting from (4.5) we obtain the simple expression for the average conductivity

$$\bar{\sigma}(\omega)=\frac{e^2}{\omega}\int d\varepsilon[f(\varepsilon')-f(\varepsilon)]\times\sum_n\delta(\sin\{\tfrac{1}{2}[V_0(\varepsilon)-V_0(\varepsilon')-n\tau]\})\times e^{-2\gamma|n|}\sin^2(\mu n)\ . \tag{4.6}$$

The term with $n=0$ vanishes so that the dc conductivity is zero. We discuss this formula firstly at $T=0$ K and then at finite temperature.

A. $T=0$ K

Introducing the variable $\varepsilon''=\varepsilon-\mu-\omega/2$, where μ is the Fermi energy we then have at low frequencies

$$V_0(\varepsilon)-V_0(\varepsilon')=2\pi\omega(\rho_F+\varepsilon''\rho_F')\ , \tag{4.7}$$

where ρ_F and ρ_F' are the density of states and its derivative at the Fermi energy. In the δ function we can replace $n\tau$ by $2\pi\langle n\bar{\tau}\rangle$, where $\bar{\tau}=\tau/2\pi$ and the angular brackets indicate the fractional part. Then

$$\bar{\sigma}(\omega)=\frac{e^2}{\pi\omega}\int_{-\omega/2}^{\omega/2}d\varepsilon''\sum_n\delta[\omega(\rho_F+\varepsilon''\rho_F')-\langle n\bar{\tau}\rangle]\times e^{-2\gamma|n|}\sin^2(\mu n)\ . \tag{4.8}$$

We have replaced the sin by its argument which is small. We now evaluate this formula close to certain special frequencies ω_{k0} such that $\rho_F\omega_{k0}=q_k(\bar{\tau}-p_k/q_k)$, where p_k and q_k are the kth convergents of $\bar{\tau}$. Thus $\bar{\tau}=p_k/q_k+\delta_k$, where $\delta_k=\bar{\tau}-p_k/q_k$ and is small and positive if k is large and even and $\langle q_k\bar{\tau}\rangle=q_k\delta_k$. Substituting these results in (4.8) we find

$$\bar{\sigma}(\omega_{k0})=\frac{e^2}{\pi\rho_F'\omega_{k0}^2}e^{-2\gamma q_k}\sin^2(\mu q_k)\ . \tag{4.9}$$

This formula applies for frequencies such that

$$|\omega-\omega_{k0}|<\omega_{k0}^2\rho_F'/2\rho_F\ .$$

The conductivity thus has a series of steps at the frequencies ω_{k0} of width given above. From the inequality

$$\frac{1}{q_k(q_{k+1}+q_k)}<\delta_k<\frac{1}{q_kq_{k+1}}$$

we see that

$$\rho_F\omega_{k0}=q_k\delta_k\sim\frac{1}{q_k}\ , \tag{4.10}$$

where q_k is the spatial distance between states differing in energy by ω_{k0}. The frequency difference between successive steps is

$$\rho_F(\omega_{k0}-\omega_{k+20})=\bar{\tau}(q_k-q_{k+2})-(p_k-p_{k+2})=a_{k+2}q_{k+1}|\delta_{k+1}|\ , \tag{4.11}$$

where we have used the recursion relations for the convergents $q_k=q_kq_{k-1}+q_{k-2}$ and similarly for p_k. Thus the frequency difference between steps is of order

$$\omega_{k0}-\omega_{k+20}\sim\frac{1}{\rho_Fq_{k+1}}$$

which is larger than the width of a step.

In (4.9) using $q_k\sim1/\rho_F\omega_{k0}$ the conductivity is approximated by the continuous function

$$\bar{\sigma}(\omega)\sim\frac{e^2}{\pi\rho_F'\omega^2}e^{-2\gamma/\rho\omega}\sin^2(\mu/\rho\omega)\ . \tag{4.12}$$

The exponential dependence of the conductivity on inverse frequency at low frequencies has been obtained by Prange *et al.*[6] and Pastur and Figotin.[5] They also pointed out that the incommensurate case has a smaller conductivity than the disordered case where $\sigma\sim\omega^2$.

B. $T\neq0$ K

We consider the case where $k_BT>\omega$ but k_BT is much less than the Fermi energy μ. In (4.6) put $\varepsilon=\mu+\varepsilon''$ and expand

$$V_0(\varepsilon)-V_0(\varepsilon-\omega)=2\pi\omega(\rho_F+\varepsilon''\rho_F')\ . \tag{4.13}$$

Then (4.8) is replaced by

$$\bar{\sigma}(\omega)=\frac{e^2}{4\pi k_BT}\int d\varepsilon''\frac{1}{\cosh^2(\beta\varepsilon''/2)}\sum_n\delta((\rho_F+\varepsilon''\rho_F')\omega-\langle n\bar{\tau}\rangle)e^{-2\gamma|n|}\sin^2(\mu n)\ . \tag{4.14}$$

The integral is effectively over the interval $|\varepsilon''| < k_B T$ which broadens the steps at the special frequencies ω_{k0}. From (4.14)

$$\bar{\sigma}(\omega_{k0}) = \frac{e^2}{4\pi\rho_F' k_B T \omega_{k0}} e^{-2\gamma q_k} \sin^2(\mu q_k) ,$$

which replaces (4.9) in the case $k_B T > \omega$. This formula applies for frequencies

$$|\omega - \omega_{k0}| < \frac{\omega_{k0} k_B T \rho_F'}{\rho_F} .$$

Thus the steps are broadened by temperature and the conductivity is temperature dependent $\sigma \sim T^{-1}$. Such a behavior has been discussed recently for systems with localized states by Azbel *et al.*[7] The width of steps will only be comparable with the distance between steps, i.e.,

$$\omega_{k0} k_B T \rho_F' \sim \rho_F |\omega_{k0} - \omega_{k+20}| = a_{k+2} q_{k+1} |\delta_{k+1}| \sim \rho_F \omega_{k0} , \quad (4.15)$$

where we have used $q_{k+1}\delta_{k+1} \sim 1/q_{k+1} \sim \rho_F \omega_{k0}$. This gives $k_B T \sim \rho_F/\rho_F'$ a high temperature. Thus the steps or resonances in the ac conductivity are not readily smoothed out by finite temperatures. However, we have not considered inelastic effects which would be expected to become important before the above temperature is reached. These are discussed in Sec. V.

V. HOPPING CONDUCTIVITY

The model (1.1) and the conductivity in Sec. IV only take elastic scattering of the electrons into account. At finite temperatures inelastic effects will be important and eventually dominate the conductivity. We have not attempted to include inelastic scattering in (1.1) in any detailed way but will attempt to treat it in the same way as is done in disordered systems.[7] The phonon-assisted hopping rate W_{ij} between localized states of energies ε_i and ε_j at positions R_i and R_j is taken to be

$$W_{ij} = V e^{-\gamma |R_i - R_j| - |\varepsilon_i - \varepsilon_j|/k_B T} , \quad (5.1)$$

where V is a constant dependent on the electron-phonon coupling and γ is the localization length defined in (2.13). In the case where $\tau/2\pi$ is the golden mean the distribution of localized states in energy and position has been discussed above (2.13). Substituting these results in (5.1) we find for two states a distance f_p apart

$$W_{f_p} = V e^{-\gamma f_p - 1/k_B T \rho f_p \sqrt{5}} \quad (5.2)$$

so that W_{f_p} only depends on the distance between the two sites. In this case the motion of the electrons can be defined by a simple master equation

$$\frac{dP_i}{dt} = \sum_j W_{ij}(P_j - P_i) , \quad (5.3)$$

where P_i is the probability of finding the electron in site i. The diffusion constant is given by

$$D = \tfrac{1}{2} \sum_j (i-j)^2 W_{ij} . \quad (5.4)$$

We maximize the hopping probability W_{f_p} with respect to f_p and find that the most probable transition is for $f_p^* = (\sqrt{5} k_B T \rho \gamma)^{-1/2}$ and

$$W_{f_p^*} = V e^{-(T_0/T)^{1/2}} , \quad (5.5)$$

where $T_0 = \gamma/\kappa\rho\sqrt{5}$. This result is exactly the same as the Mott law[8] for hopping conductivity in disordered systems. A more accurate formula for the diffusion constant can be obtained from (5.4).

The crossover between resonance tunneling conductivity considered in Sec. IV and phonon-assisted hopping conductivity will occur when the length f_p^* for the most probable hop becomes less than the distance $q_k \sim 1/\rho\omega_{k0}$ needed to tunnel to find a resonant state with frequency difference ω_{k0}. Setting these two lengths equal (ignoring numerical factors) gives a relation between temperature and frequency

$$k_B T \gamma \sim \rho \omega^2 \quad (5.6)$$

at which this crossover should occur. We have derived the Mott law for incommensurate systems in the case of the golden mean but we would expect the same result to hold for ordinary irrational τ

VI. TRANSMISSION COEFFICIENT

In this section we discuss the transmission of an incident electron wave of energy $\varepsilon = 2W\cos k$ through a one-dimensional incommensurate system of length L described by (1.1). We suppose that the incommensurate lattice is connected at each end to a perfect lattice and the sites of the incommensurate lattice are labeled 1 to L. The transmission coefficient T_L is related to the conductance G_L by the Landauer[9] formula

$$G_L = \frac{e^2}{2\pi\hbar} \frac{T_L}{1 - T_L} . \quad (6.1)$$

In the Appendix we express the transmission coefficient in terms of the Green's function (3.9) at energy ε:

$$T_L = \frac{4\sin^2 k}{W^2} \left| \frac{G_{0L+1}}{D} \right|^2 , \quad (6.2)$$

where

$$D = (G_{10} - e^{-ik} G_{00})(e^{ik} G_{LL+1} - G_{L+1L+1}) + (e^{-ik} G_{0L+1} - G_{1L+1})(e^{ik} G_{L0} - G_{L+10}) . \quad (6.3)$$

G is the Green's function for the infinite system and is expressed in (3.9) in terms of the eigenstates of the infinite system. Equation (6.2) is an exact formula for the transmission coefficient of a finite system of length L. As the eigenstates are exponentially localized, the eigenstates of the finite system will not differ much from those of the infinite system except close to the boundaries. We will find that the transmission due to states close to the boundaries is small and, thus, (6.2) is an appropriate for-

mula for the discussion of the transmission coefficient.

For energies ε not near resonance with a localized state, the Green's function in the numerator of (6.2) decreases exponentially with L like $G_{0L}\sim e^{-\gamma L}$ while in the denominator D the Green's functions G_{00}, G_{LL+1}, etc., do not decrease with L. Thus, as expected, $T_L\sim e^{-2\gamma L}$ when we are not near a resonance.

We now investigate how T_L behaves when ε is very close to resonance with a localized mode of energy ε_ν located at $\nu(1<\nu<L)$. ε_ν is related to ν by (2.8). We can now write the Green's function as the sum of two parts, the first coming from the nearly resonant mode and the remainder

$$G_{mn}=c_m c_n\cot\{\tfrac{1}{2}[\alpha-V_0(\varepsilon)-\nu\tau]\}F_{m-\nu}F_{n-\nu}+G'_{mn} \quad (6.4)$$

and using $\alpha-\nu\tau+2\pi l=V_0(\varepsilon_\nu)$ for ε close to ε_ν we can write this as

$$G_{mn}=g^{(\nu)}_{mn}/\delta_\nu+G'_{mn}\ , \quad (6.5)$$

where $\delta_\nu=\varepsilon_\nu-\varepsilon$ and

$$g^{(\nu)}_{mn}-c_m c_n F_{m-\nu}F_{n-\nu}/\pi\rho\ .$$

We now substitute (6.5) in (6.2). It should be noted that the terms in δ_ν^{-2} cancel in the denominator D and we find

$$T_L=\frac{4\sin^2 k}{W^2}\left|\frac{g^{(\nu)}_{0L+1}+\delta_\nu G'_{0L+1}}{A+\delta_\nu B}\right|^2 , \quad (6.6)$$

where

$$A=(g^{(\nu)}_{10}-e^{-ik}g^{(\square)}_{00})(e^{ik}G'_{LL+1}-G'_{L+1L+1})$$
$$+(G'_{10}-e^{-ik}G'_{00})(e^{ik}g^{(\nu)}_{LL+1}-g^{(\nu)}_{L+1L+1})\ , \quad (6.7)$$

$$B=(G'_{10}-e^{-ik}G'_{00})(e^{ik}G'_{L+1L}-G'_{L+1L+1})\ . \quad (6.8)$$

In A and B we have omitted exponentially small terms $\sim e^{-\gamma L}$. In order to exhibit the important features of (6.6) we make the following simplifying but reasonable assumptions. (a) The state ν of interest is located deep inside the incommensurate system $1\ll\nu\ll L$ and set $\nu=L/2+\nu'$. (b) The wave functions $F_\nu\sim e^{-\gamma\nu}$, $F_{L-\nu}\sim e^{-\gamma(L-\nu)}$, and thus $g^{(\nu)}_{10}\sim g^{(\nu)}_{00}\sim e^{-2\gamma\nu}/\rho$ and $g^{(\nu)}_{LL+1}\sim g^{(\nu)}_{L+1L+1}\sim e^{-2\gamma(L-\nu)}/\rho$ and neglect all phase factors. (c) The Green's functions $G'_{10}\sim G'_{00}\sim G'_{L+1L}\sim G'_{L+1L+1}$ are all of order G' independent of L. With these assumptions $g^{(\nu)}_{0L+1}\sim e^{-\gamma L}/\rho$, $A\sim e^{-\gamma L}\cosh 2\gamma\nu' G'/\rho$ and $B\sim(G')^2$ and the transmission coefficient has the form

$$T_L\sim\left|\frac{1}{\cosh 2\gamma\nu'+\delta_\nu\rho G' e^{\gamma L}}\right|^2 . \quad (6.9)$$

This formula shows that the width of the resonances in T_L due to localized states is proportional to $e^{-\gamma L}$. Exactly at resonance, $\delta_\nu=0$, the transmission coefficient is proportional to $1/\cosh^2 2\delta\nu'$ and then localized states located near the center of the wire ($\nu'\sim 0$) give the largest contribution and states near the edges ($\nu'=\pm L/2$) give a negligible contribution to the transmission. These results are in general agreement with those expected for disordered systems as discussed by Azbel and Soven,[10] Azbel,[11] and Maynard and Akkermans.[12] DeVincenzo and Azbel[13] have discussed the temperature dependence of the conductance in this case and the crossover to a Mott-like law. The conductance at finite temperatures is given by

$$G=\frac{e^2}{2\pi\hbar}\int d\varepsilon\left[-\frac{\partial f}{\partial\varepsilon}\right]T_L(\varepsilon)\ , \quad (6.10)$$

where f is the Fermi function. Since T is exponentially large at the resonances, the integral is dominated by the resonances and the contribution of a resonance ε_ν at site ν (measured from the center of wire) is

$$G\sim-\left[\frac{\partial f}{\partial\varepsilon}\right]\delta\varepsilon_\nu T_L(\varepsilon_\nu)=e^{-\gamma L-2\gamma|\nu|-2\beta|\varepsilon_\nu-\mu|}\ , \quad (6.11)$$

where $\delta\varepsilon_\nu\sim e^{-\gamma L}$ is the width of the resonance, $e^{-2\gamma|\nu|}$ is the value of T at resonance and the third factor comes from the Fermi function. Suppose that the chemical potential μ is approximately in resonance with a state ε_{ν_0}, where ν_0 is near the center of the sample. Then maximizing (6.11) with respect to ν assuming $(\varepsilon_\nu-\mu)\sim 1/\rho|\nu|$ we find $G\sim e^{-\gamma L-(T_0/T)^{1/2}}$, where T_0 is the same as in the phonon-assisted case (5.5). The temperature dependence is the same as in the Mott hopping law.

VII. DISCUSSION

We have discussed three types of conductivity (a) resonant tunneling (Sec. IV), (b) phonon-assisted hopping (Sec. V), and (c) transmission through a system of finite length. Each of these involves a length scale: (a) For resonant tunneling the length scale is set by the frequency and is of order $1/\rho\omega$, (b), for phonon-assisted hopping the length scale is set by the distance for the most probable hop $(k_B T\rho\gamma)^{-1/2}$ and (c) for transmission the size L of the system sets the scale. The relative values of these three length scales determines the type of conductivity expected the shortest length scale being the dominant one.

The incommensurate model of Grempel, Fishman, and Prange[1] provides a simple example in which the different types of transport processes occurring in incommensurate systems with localized states can be investigated in some detail.

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APPENDIX

We derive an expression for the transmission coefficient of an incident electron wave of energy $\varepsilon=2W\cos k$ through a one-dimensional incommensurate system of length L described by

$$(t_m-\varepsilon)a_m+W(a_{m+1}+a_{m-1})=0\ . \quad (A1)$$

We suppose the incommensurate lattice occupies the sites 1 to L and is connected at each end to a perfect lattice ($t_m=0$). We thus require a solution of (A1) such that

$$a_m = \begin{cases} e^{ikm} + re^{-ikm}, & m < 1 \\ te^{ikm}, & m > L \end{cases} . \tag{A2}$$

Let $G_{m,n}$ be the Green's function for the infinite incommensurate system which includes the piece L of interest. Then

$$a_m = \alpha G_{m,n_1} + \beta G_{m,n_2}, \quad 2 < m < L-1 \tag{A3}$$

where $n_1 < 1$ and $n_2 > L$. From (A2) and (A3) we see that (A1) is satisfied for (i) $m < 0$; (ii) $m > L+1$; (iii) $3 < m < L-2$. We are left with the four equations (A1) for $m = 1$, 2, $L-1$, and L. Substituting (A2) and (A3) in these equations provides four equations for the unknowns r, t, α, and β. After some algebra we find

$$t = 2i \sin(k) e^{-ikL} \frac{N_{n_1 n_2}}{D_{n_1 n_2}} , \tag{A4}$$

where

$$N_{n_1 n_2} = G_{Ln_1} G_{L-1,n_2} - G_{L-1,n_1} G_{Ln_2} , \tag{A5}$$

$$\begin{aligned} D_{n_1 n_2} = & [G_{1n_1} - e^{-ik}(G_{0n_1} - \delta_{1,n_1})] \\ & \times (e^{ik} G_{Ln_2} - G_{L+1,n_2} + \delta_{1,n_2}) \\ & + (e^{-ik} G_{0n_2} - G_{1n_2})(e^{ik} G_{Ln_1} - G_{L+1,n_1}) . \end{aligned} \tag{A6}$$

The index n_1 must be to the left and n_2 to the right of the incommensurate system but are otherwise arbitrary. We have conveniently chosen them to be $n_1 = 0$, $n_2 = L+1$ which eliminates the δ function in (A6).

The numerator (A5) can be simplified by using the identity

$$W(G_{m+1,n_1} G_{mn_2} - G_{m+1,n_2} G_{mn_1}) - W(G_{mn_1} G_{m-1,n_2} - G_{mn_2} G_{m-1,n_1}) = \delta_{m,n_1} G_{mn_2} - \delta_{m,n_2} G_{mn_1} . \tag{A7}$$

We can write

$$N_{0L+1} = G_{L0} G_{L-1,L+1} - G_{L-1,0} G_{L,L+1} = G_{m0} G_{m-1,L+1} - G_{m-1,0} G_{m,L+1}, \quad 0 < m < L+1 . \tag{A8}$$

If we now use the formula (A7) to shift m to $\pm\infty$ we pick up a contribution from one of the δ functions in (A7) and the remainder vanishes as $m \to \pm\infty$. Thus

$$N_{0,L+1} = W^{-1} G_{0,L+1} . \tag{A9}$$

Substituting (A6) and (A9) in (A4) gives (6.2).

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