Reentrant localization and a mobility gap in superlattice minibands

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We develop a theory of the mobility edge for transport in superlattice minibands. For small W, where $2W$ is the bandwidth, the mobility edge E_c diverges as $\ln 1/W$, so that all states are localized in the limit $W \to 0$. For large values of W, we find $E_c \sim 1/W$, and the system behaves as an anisotropic conductor. For intermediate values of W, the system can develop a mobility gap—a band of localized states—at the Van Hove singularity in the density of states. This reentrant localization behavior should be experimentally observable and may explain some recent experimental results.

In recent years, the physics of electronic transport in superlattices has become a topic of intense experimental and theoretical investigation.[1] Theoretical studies have focused on a number of issues affecting the mobility of carriers in these systems, such as electron-phonon[2] and electron-impurity scattering.[3,4] On the experimental side, recent work has clearly demonstrated that Bloch transport perpendicular to the superlattice layers (i.e., vertical transport) can take place in sufficiently high-quality samples.[5,6] One topic of particular interest to both experimentalists and theorists in this area is the localization properties of these systems.[1,4,7] In particular, by varying the bandwidth $2W$, one may take the system from an essentially anisotropic three-dimensional system ($2W \gg E_F$) to a set of disconnected two-dimensional systems ($2W = 0$). It is believed that in the presence of any disorder, all states in two dimensions should be localized.[8] Conversely, in a three-dimensional system one expects there to be a mobility edge—i.e., a unique energy E_c separating localized and extended states.[8,9] In what follows, we will consider how transport properties of a superlattice interpolate between these two limits as a function of $2W$. We will find that, under suitable (and experimentally attainable) conditions, this system can exhibit reentrant localization, characterized by a mobility gap in the spectrum. This mobility gap, which is the interesting new result in this paper, arises from a subtle interplay between the peculiar band structure of a superlattice and the quantum interference effect responsible for producing Anderson localization. To the best of our knowledge this is the first known example of nontrivial band-structure effects on localization.

In our model, we work within a single miniband of the superlattice, whose dispersion relation in the absence of impurities has the form $\varepsilon(\mathbf{k}) = k_\parallel^2/2m + (W - W\cos k_z a)$, where $\mathbf{k}_\parallel = (k_x, k_y)$, a is the superlattice period, and $2W$ is the miniband width. (In all of what follows, we set $\hbar = 1$.) This model is essentially an extremely anisotropic *three-dimensional* system. Our general approach is to evaluate the Kubo formula for the conductivity approximately in terms of the diffusion constants $D_{\parallel(z)}$ for motion parallel (perpendicular) to the planes; with the Einstein relations, this generates a set of self-consistent equations.[10] The metal-insulator transition (MIT) is then found by taking the limit $D_{\parallel(z)} \to 0$.

For general values of the bandwidths, we must solve for the mobility edge numerically. Figure 1(a) shows an example of our results for $\lambda = 0.4$, where λ characterizes the strength of the impurity potential, and is proportional to the impurity density,[11] and lengths here are measured in units of a and energies in units of $1/ma^2$. The most striking results are the multivalued solutions, indicating reentrant localization, in the range $0.11 < W < 0.13$. In Fig. 1(b) we illustrate the density of states along with the mobility edges when W is in this regime. As usual, the lowest-energy states near the band edge are localized; however, we see that *there is a novel band of localized states near the Van Hove singularity at* $E = 2W$. We should expect that, as a function of Fermi energy, the conductivity will vanish over this range of energies; thus, the system displays a mobility gap in this range.

To understand the physical origin of this mobility gap, one need only examine the shape of the Fermi surface for various carrier densities, as illustrated in Fig. 2. In momentum space, the points $\mathbf{k} = (0, 0, \pm\pi/a)$ are critical points that lead to the cusp in $N(E_F)$ at $E_F = 2W$. As the Fermi surface approaches these points, there is a sudden increase in the density of states, causing an enhancement of the scattering rate when $E_F \sim 2W$. Within our approximations, for large enough λ, the enhancement is sufficient to localize a band of states.[12,13] We emphasize that because of this mechanism, a more detailed treatment of this problem (i.e., one that includes all contributions to the vertex function, electron-electron interactions, other kinds of scattering potentials, etc.) must also lead to a suppression of the mobility for $E_F \sim 2W$.

We believe that a mobility gap in such systems should be experimentally observable. The parameters needed to produce a sample with a mobility gap should be relatively easy to achieve; for example, within our theory, a GaAs-$Al_xGa_{1-x}As$ sample with $a = 60$ Å would require $2W \simeq 3.0$ meV to achieve a mobility gap for heavy holes, if we estimate the elastic scattering rate to be $1/2\tau = 2W$. Such system parameters are quite reasonable for present-

day superlattices. Furthermore, as we will discuss below, the presence of a mobility gap would explain some recent experimental observations by Fujiwara *et al.*[2] that are not presently well understood.

There are two limits in which we can obtain approximate analytic expressions for the mobility edge. When $W \to 0$, we find $E_c \simeq (2\lambda m/\pi a)\ln\Gamma_0/W$, where $\Gamma_0 = 1/2\tau$ is the imaginary part of the self-energy and τ is the elastic scattering lifetime. This solution is illustrated in Fig. 1(a). The logarithmic divergence with W indicates that for vanishing bandwidth, all the states are localized. This is reasonable, because the limit $W \to 0$ represents the one in which coupling between layers becomes negligible, leading to a set of independent two-dimensional systems. This divergence is analogous to the logarithmic singularity one finds when computing the low-frequency conductivity of a two-dimensional system. Indeed, the bandwidth W plays a role very similar to that of the frequency for a two-dimensional system; it provides an infrared cutoff that would otherwise lead to a divergence in the vertex corrections to the conductivity.

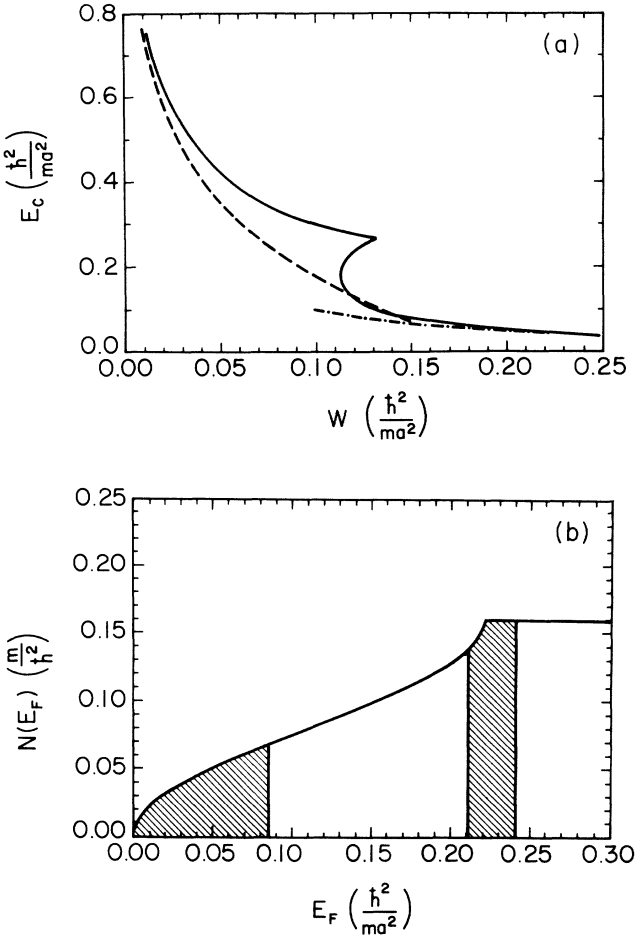

FIG. 1. (a) Mobility edge as a function of the half bandwidth, W. Solid line, numerical results; dashed line, analytic result for small W; dashed-dotted line, analytic result for large W. (b) Density of states showing mobility edges when W is in the regime for which E_0 is multivalued. Shaded areas denote bands of localized states, solid areas are extended states.

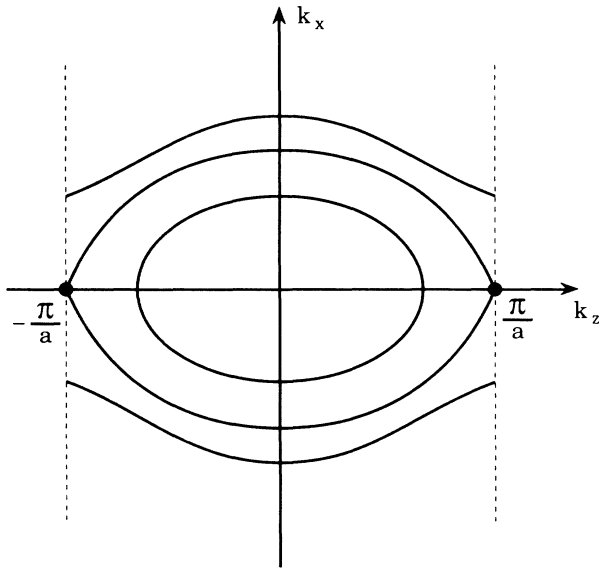

FIG. 2. Fermi surfaces for several values of E_F. The points $k_z = \pm\pi/a$ are critical points.

The other limit that we may understand analytically is that of a large bandwidth ($W \gg \Gamma_0$). In this case, we find $E_c \simeq 0.0623(\lambda/ma)^2 W$; the mobility edge vanishes as $W \to \infty$. The result is sensible when we realize that this is the limit of a highly anisotropic conductor, with an effective mass in the z direction given by $m_z = 1/Wa^2$. Thus, $W \to \infty$ corresponds to infinitely light carriers, which cannot be localized. The analytic form is shown for $\lambda = 0.4$ in Fig. 1(a); the result agrees quite well with the numerical solution for $W > 0.175$.

We begin our analysis with the $T = 0$, zero-frequency Kubo formula, in the form[14] $\sigma_{\mu\nu} = \sigma^{\mathrm{I}}_{\mu\nu} + \sigma^{\mathrm{II}}_{\mu\nu}$, where

$$\sigma^{\mathrm{I}}_{\mu\nu} = \frac{e^2}{\pi}\int \frac{d^3k}{(2\pi)^3} v_\mu(\mathbf{k}) v_\nu(\mathbf{k}) |G^R(E_F,\mathbf{k})|^2 , \tag{1a}$$

$$\sigma^{\mathrm{II}}_{\mu\nu} = \frac{e^2}{\pi}\int \frac{d^3k d^3k'}{(2\pi)^6} v_\mu(\mathbf{k}) v_\nu(\mathbf{k}') \times |G^R(E_F,\mathbf{k})|^2 \Gamma(\mathbf{k},\mathbf{k}') |G^R(E_F,\mathbf{k}')|^2 . \tag{1b}$$

Here, $v_\mu(\mathbf{k}) = \partial\varepsilon/\partial k_\mu$, $G^R(E_F,\mathbf{k}) \simeq [E_F - \varepsilon(\mathbf{k}) + i\Gamma_0]^{-1}$ is the retarded Green's function, Γ_0 is the imaginary part of the self-energy (which has been calculated previously[3]), and $\Gamma(\mathbf{k},\mathbf{k}')$ is the four-leg vertex function. We note that if one ignores the vertex corrections (σ^{II}), our formula reduces to that used by Yang and Das Sarma.[3] In our theory, we express $\Gamma(\mathbf{k},\mathbf{k}')$ in terms of an irreducible vertex function $U(\mathbf{k},\mathbf{k}')$. This is the sum of all diagrams that cannot be broken into disconnected parts by cutting two Green's-function lines; the relationship between the two quantities is

$$\Gamma(\mathbf{p},\mathbf{q})=U(\mathbf{p},\mathbf{q}) + \int \frac{d^2p'}{(2\pi)^3} U(\mathbf{p},\mathbf{p}')|G^R(E_F,\mathbf{p}')|^2\Gamma(\mathbf{p}',\mathbf{q}) .$$

To proceed, we use an approximate form for U, given by

$$U(\mathbf{k},\mathbf{q})=\frac{2\lambda\Gamma_0}{D_\parallel(\mathbf{q}_\parallel+\mathbf{k}_\parallel)^2+D_z(q_z+k_z)^2} . \quad (2)$$

This expression is just the sum of the maximally crossed diagrams, evaluated for small momentum transfer $|\mathbf{q}+\mathbf{k}|$, where we have replaced the zeroth-order diffusion constants with their values renormalized by vertex corrections.[10,15] This procedure is sensible near the MIT, where the vertex corrections are very pronounced. Noting that $U(\mathbf{k}+\mathbf{q})$ strongly favors backscattering of electrons, we replace $v_\nu(\mathbf{k}')$ with $v_\nu(-\mathbf{k})$ in Eq. (1b);[4] we can then combine Eqs. (1)–(3) with the Einstein relations $\sigma_{\parallel(z)}=e^2N(E_F)D_{\parallel(z)}$ to generate two self-consistent equations for the diffusion constants:

$$D_\mu N(E_F)\cong\frac{1}{\pi}\int\frac{dk_z}{2\pi}\frac{g_1^\mu(k_z)}{1+J(k_z)} , \quad (3)$$

where

$$g_1^\mu(k_z)=\int\frac{dk_xdk_y}{(2\pi)^2}|v_\mu(\mathbf{k})|^2|G^R(E_F,\mathbf{k})|^2 ,$$
$$J(k_z)=\int\frac{d^3q}{(2\pi)^3}|G^R(E_F,\mathbf{q}-\mathbf{k})|^2U(\mathbf{q},0) . \quad (4)$$

The k_z momentum in these expressions parametrizes the Fermi surface. To find the mobility edge, we divide Eqs. (4) by D_μ, and take the limit $D_\mu\to 0$. One is then left with two equations for the parameters $r=D_z/D_\parallel$ and E_c, where E_c is the value of E_F satisfying these equations; i.e., the mobility edge. We note that in order to perform the integral in Eq. (4), we must expand the Green's function for small $q_\parallel$, and introduce an elastic scattering cutoff wave vector q_0. The choice of this cutoff is somewhat subtle,[13] but the most natural choice is the inverse elastic scattering length. With this in mind, we set $q_0^2=2m\Gamma_0$.

As a specific example, we can perform the integration in Eq. (4) in the limit $W\ll\Gamma_0\ll E_F$. In this situation, $J(k_z)$ is approximately independent of k_z; the self-consistent equation for the mobility edge then takes the simple form $D_\mu J=D_\mu^0$. From this, it is clear that the ratio $r\equiv D_z/D_\parallel=D_z^0/D_\parallel^0\equiv r_0$, as has been noted by Szott *et al.*,[4] where D_z^0 and $D_\parallel^0$ are the diffusion constants computed without vertex corrections. This is a considerable simplification, because we can explicitly compute r_0 using $D_z^0/D_\parallel^0=\sigma_z^1/\sigma_\parallel^1$. Equation (4) may then be evaluated in the small-W limit; we find for the mobility edge $E_c\simeq(2\lambda m/\pi a)\ln(\Gamma_0/W)$, where $\Gamma_0\simeq\lambda m/2a$. This analytic form gives reasonable agreement with our numerical result for very small values of W.

The analytic solution in the small-W limit is possible because the Fermi surface is nearly cylindrical in this situation. In a different limit, $E_F\ll W$, the Fermi surface is nearly ellipsoidal; in this case, a change of variables in the $\hat{\mathbf{z}}$ direction allows us to map the relevant integrals onto ones with a spherical Fermi surface. In this case, we may also find the mobility edge analytically. It is convenient to reformulate the analysis in spherical rather than polar coordinates: one finds, after an analysis similar to that above, $E_c=(\lambda m/a)^2y_0/W$, with $y_0=0.0623$.

Unfortunately, one cannot evaluate the integrals in Eqs. (3) and (4) analytically for the general case. To find E_c over the entire range of W, we have solved these equations numerically. For every value of W, we find the ratio $r=D_z/D_\parallel$ and E_c using an iterative technique. Convergence can usually be achieved within five iterations. It is interesting to note that, for all the system parameters we tested, when $r_0<1$, one finds that r and r_0 are virtually identical. We have no general proof that this should be the case; indeed, in the (unphysical) regime $r_0>1$, we find significant deviations between the two quantities, suggesting that they may not be the same in general. We note that for $W\ll E_F$ and $W\gg E_F$, one can show $r\simeq r_0$.

The most surprising of our results is that for $\Gamma_0\cong W$ one finds that E_c may be multivalued, which indicates the presence of a mobility gap. As explained above, the effect may be understood in terms of the critical points in the Brillouin zone; when the Fermi energy approaches $2W$, there is a sudden increase in the density of states that allows for an enhanced scattering rate of the electrons. The impurity density and bandwidth $2W$ must be adjusted properly for this effect to occur. The mechanism inducing the mobility gap, however, always occurs near the Van Hove singularity, so that even if the parameters are not adjusted properly to induce localization in this energy regime, one should still find a reduction in the mobility.

Finally, we note that this effect may explain some experimental findings of Fujiwara *et al.*[6] In this experiment, the mobilities of holes in an $a=50$ Å superlattice were measured indirectly. The authors observed two peaks in the photoluminescence spectrum, which they associate with recombination of electrons with heavy holes and light holes, respectively, within the superlattice. The relative weights of the peaks as a function of temperature are then an indirect measure of the dwell time of the holes in the superlattice. They find a monotonically decreasing peak height with temperature for the light holes, whereas the heavy-hole peak *first increases, then decreases* as the temperature is raised. This suggests that the heavy-hole mobility initially decreases with temperature, then increases. In our model, this can be explained if the Fermi energy for the heavy holes lies in a band of extended states below either a mobility gap, or a band of states with reduced mobility. As the temperature is raised from $T=0$, the electrons will begin to populate the states in this band, and only at higher temperatures occupies conducting states. Our estimates using the bandwidth $2W$ quoted by the authors, and assuming the elastic scattering rate is roughly of the order of $2W$, gives an energy scale of approximately 40 K for the size of the mobility gap, which is consistent with their data. We note, however, that an experiment of this kind only indicates a decrease in the mobility over a certain energy range; it cannot tell us whether the states in this range are actually localized.

In conclusion, we have developed a theory of the mobility edge in a superlattice miniband. We discover that the band structure may have a very interesting effect (i.e., reentrant localization) on the localization properties of this system. The presence of a mobility gap, or at least a reduction in the mobility over a range of energies, can explain some recent experimental findings.[2] Finally, it is important to emphasize that effects neglected in this paper (e.g., electron-electron interactions, higher-order impurity scattering diagrams, more-realistic impurity potential), while modifying the details of our results, are unlikely to change our central conclusions, namely the existence of either a mobility gap or a band of reduced mobility states, because these follow from the enhanced scattering at the Van Hove singularity.

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