Valley Fluctuations in Degenerately Doped Semiconductors

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(Received 18 December 1986)

The valley quantum number of electrons in the conduction band of doped semiconductors is shown to affect the electron dynamics in a manner analogous to the spin quantum number. Recent theoretical and experimental studies have demonstrated the strong effects of disorder-enhanced electron-electron interactions upon the spin susceptibility and electron-spin-resonance spectrum. It is shown that similar effects should also exist in the valley fluctuations, leading to measurable consequences in the ultrasonic attenuation at low temperatures.

PACS numbers: 71.30.+h, 62.80.+f, 72.50.+b, 76.30.Lh

Degenerately doped semiconductors have been used extensively to study the properties of interacting electrons in a random potential.[1,2] Conductivity measurements have shown that the electrons undergo a continuous metal-insulator transition at a certain critical density of doping.[1] Recent theoretical analyses[3-7] have pointed out the importance of electron-spin fluctuations upon the metallic side of the metal-insulator transition. An enhancement of the spin susceptibility and a suppression of the spin-diffusion coefficient over the corresponding quantities for charge fluctuations have been predicted at low temperatures. Trends in accord with these expectations have been observed in an electron-spin-resonance experiment in phosphorus-doped silicon.[6-8] In this paper we focus attention upon the *many-valley* nature of the semiconductor conduction band. The additional valley quantum number is shown to alter the electron dynamics in a manner which is analogous to that due to the spin degeneracy. This similarity between the spin and valley quantum numbers was recently recognized in an entirely different context in the quantized Hall effect by Rasolt, Halperin, and Vanderbilt.[9] Just as was the case with spin fluctuations, the interaction of long-wavelength and long-time diffusive valley fluctuations leads to an enhancement of the appropriately defined "valley susceptibility" and a corresponding suppression of the "valley diffusion" constant at low temperatures.

I argue in this paper that ultrasound experiments in degenerately doped semiconductors can be used to probe the effects of the interacting valley fluctuations. As is well known,[10,11] the dominant effect of the dopant electrons upon the propagation of ultrasound is through processes involving transfer of electrons between conduction-band valleys. The oscillating shear strain in an ultrasonic wave lifts the degeneracy between the valleys. By use of the spin analogy, the shear strain is similar to a magnetic field which lifts the degeneracy between up and down spins. We can therefore use the techniques developed for evaluating magnetic response functions to calculate changes in the velocity and attenuation of the ultrasonic wave. It is shown below that at very low temperatures (below 1 K), the interacting valley fluctuations lead to a strong temperature dependence in the ultrasonic attenuation. This temperature-dependent attenuation should be measurable under suitable conditions in a many-valley semiconductor like silicon. Previous analyses[12] of the attenuation did not have the benefit of Finkelstein's renormalization scheme[3,4] and do not agree with my results.

The analysis in this paper will be presented with particular reference to the experimentally interesting case of silicon. The form of the results, however, is more general and should be applicable, with minor changes, to other many-valley semiconductors. The dynamics of the conduction-band electrons is described by the model Hamiltonian $H = H_0 + H_{\text{imp}} + H_{ee}$ as a sum of free electron, impurity scattering, and electron-electron interaction parts. $H_0 = \sum_{i,\sigma} \epsilon_i(\mathbf{k}) c^\dagger_{\mathbf{k}i\sigma} c_{\mathbf{k}i\sigma}$ describes free electrons moving in the six conduction-band valleys of silicon. The index i extends over the six valleys located on the $+x$, $-x$, $+y$, $-y$, $+z$, and $-z$ axes, and the index σ sums over spin-up and spin-down states. The band structure $\epsilon_i(\mathbf{k})$ is approximated by an anisotropic parabolic dispersion with differing longitudinal and transverse masses. This mass anisotropy will turn out to be of great importance later in this paper.

H_{imp} describes the scattering of the electrons from the donor atoms in the silicon crystal. The dominant scattering process is the *intra*valley process. This is modeled by an s-wave scattering potential v. It leads to an intravalley scattering rate $1/\tau_0 = 2\pi N_1 v^2$, where N_1 is the single-electron, single-spin, and single-valley density of states at the Fermi level. The donor core potentials also lead to *inter*valley scattering. The symmetry of the silicon lattice divides these processes into two types: (i) those between *collinear* valleys (e.g., between the valleys along the $+x$ and $-x$ axes) which is modeled by a scattering potential u_{xx}, and (ii) those between *noncollinear* valleys which is modeled by a scattering potential u_{xy}. These processes lead to the intervalley scattering rates $1/\tau_1 = 2\pi N_1 u_{xx}^2$ and $1/\tau_2 = 2\pi N_1 u_{xy}^2$. The relationship $\tau_0^{-1} \gg \tau_1^{-1}, \tau_2^{-1}$ is always satisfied by at least two orders of magnitude. All impurity spin-flip scattering rates are much smaller and can safely be neglected. The total single-particle lifetime τ is given by $1/\tau = 1/\tau_0 + 2/\tau_1 + 4/\tau_2$.

H_{ee} describes the Coulomb interactions between the electrons. Following Ref. 4, the interactions are represented by the Landau Fermi-liquid-like parameters $\tilde{\Gamma}_1$, $\tilde{\Gamma}_2$, and $\tilde{\Gamma}_3$ as shown in Fig. 1. $\tilde{\Gamma}_1$ and $\tilde{\Gamma}_3$ represent the direct interactions between particle-hole pairs in collinear and noncollinear valleys, respectively. The bare values of these interaction parameters are equal but they will renormalize differently. $\tilde{\Gamma}_2$ represents the exchange interaction between particles and holes in collinear valleys. All other interactions are either irrelevant for the long-wavelength physics, or much smaller in magnitude.[9] I emphasize here the following properties of the interaction parameters: (i) They are effective interaction parameters obtained after intergrating out all the short-distance and short-time fluctuations. The inclusion of long-wavelength and long-time fluctuations will lead to a scale dependence of these parameters to be considered below. (ii) They do not as yet include the long-range part of the direct Coulomb interactions, which, as in Landau's Fermi-liquid theory, has to be treated separately. (iii) Diagonalization of the interactions in the spin and valley space leads to *three* different interaction parameters $\tilde{\Gamma}_a = 4\tilde{\Gamma}_1 - \tilde{\Gamma}_2 + 8\tilde{\Gamma}_3$, $\tilde{\Gamma}_b = -\tilde{\Gamma}_2$, and $\tilde{\Gamma}_c = 4\tilde{\Gamma}_1 - \tilde{\Gamma}_2 - 4\tilde{\Gamma}_3$. This diagonalization is analogous to the usual decomposition into singlet and triplet particle-hole pairs for the single-valley case. (iv) Since the interaction parameters only include short-distance and short-time fluctuations, they are expected to be quite insensitive to the presence of H_{imp}. Consider, therefore, a hypothetical system described by H but with $H_{\text{imp}} = 0$. This system will be characterized by the Landau parameters A_0^a and A_0^s. (Here A_0^a and A_0^s are defined such that the spin susceptibility and the compressibility have their usual Fermi-liquid form.) The relationships $\tilde{\Gamma}_a = A_0^s$, $\tilde{\Gamma}_b = A_0^a$, and $\tilde{\Gamma}_c = A_0^a$ are then satisfied.

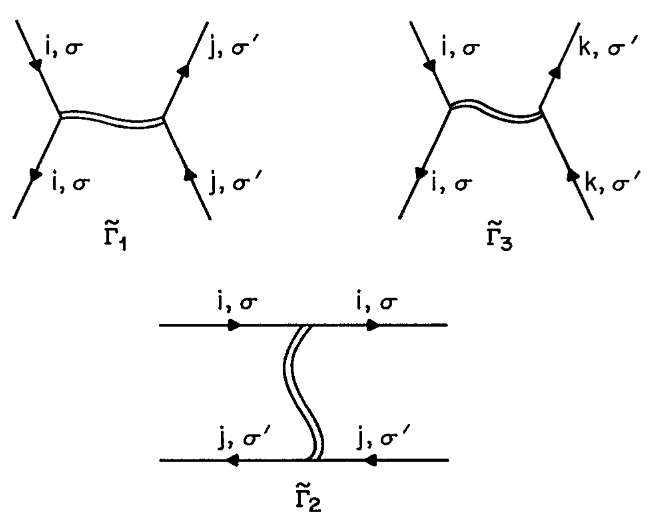

FIG. 1. The interaction parameters $\tilde{\Gamma}_1$, $\tilde{\Gamma}_2$, and $\tilde{\Gamma}_3$. They are represented by double lines to emphasize that they are *effective* parameters. Valleys j and i are collinear while valleys i and k are not.

We may now calculate particle-hole ladders.[1] They can be divided into two classes:

(i) The particle and hole carry the same valley quantum numbers [Fig. 2(a)]. These can be represented by an appropriate linear combination of L_0, L_1, and L_3, where

$$L_i = (D\mathbf{q}^2 + |\omega_n| + m_i)^{-1}.$$

Here $D = v_F^2\tau/3$ is the bare diffusion constant (v_F is a suitable average of the Fermi velocity over the Fermi surface), $m_0 = 0$, $m_1 = 2/\tau_1 + 4/\tau_2$, $m_2 = 6/\tau_2$, and $\mathbf{q}$ and ω_n are the small momentum and frequency carried by the particle-hole pair. (I am using the Matsubara finite-temperature formalism.)

(ii) The particle and hole carry *different* valley indices [Fig. 2(b)]. As pointed out by Fukuyama,[13] only when the particle and hole lie in *collinear* valleys does the particle-hole ladder yield a diffusive form. This is because the mass anisotropy causes the Fermi surfaces of noncollinear valleys to have different orientations. These ladders are given by L_3 where $m_3 = 1/\tau_1 + 4/\tau_2$.

By use of the techniques of Refs. 4–7 the renormalizations of the interaction parameters and the particle-hole ladders from diffusive electron fluctuations may be calculated. I assume that the temperature T is large enough to satisfy $\tau^{-1} \gg kT/\hbar \gg \tau_1^{-1}, \tau_2^{-1}$, because only then are the diffusive valley fluctuations important.[14] The renormalized particle-hole ladders are given by

$$L_i = \zeta^2/(D'\mathbf{q}^2 + z|\omega_n| + m_i'),$$

where I have introduced the renormalization constants z and ζ and the renormalized diffusion constant D'. The "masses" m_i' have the same form as before but with renormalized intervalley scattering times τ_1' and τ_2'. Following Castellani, Kotliar, and Lee,[15] I introduce the scaling variables $\Gamma_1 = \tilde{\Gamma}_1\zeta^2$, $\Gamma_2 = \tilde{\Gamma}_2\zeta^2$, $\Gamma_3 = \tilde{\Gamma}_3\zeta^2$, and $t = \Lambda^{d-2}/(4\pi^2 N_1 D')$ (where Λ is an upper cutoff in momentum space), and obtain the following renormal-

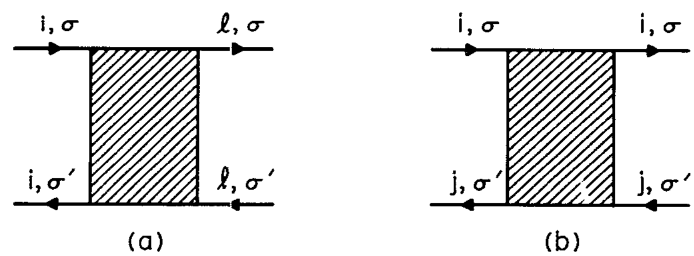

FIG. 2. The two classes of particle-hole ladders: (a) Valleys i and l can either be collinear or noncollinear. The ladder is given by a linear combination of L_0, L_1, and L_2. (b) Valleys i and j are collinear and the ladder is given by L_3.

ization-group equations in $(2+\epsilon)$ dimensions:

$$\frac{d\Gamma_1}{d\xi}=t\left[\Gamma_2+\frac{\Gamma_2^2}{z}\right],\quad \frac{d\Gamma_2}{d\xi}=t\left[\frac{1}{12}(1-A_0^g)+\Gamma_1+\frac{4\Gamma_2^2}{z}\right],\quad \frac{d\Gamma_3}{d\xi}=0,$$
$$\frac{dz}{d\xi}=-t\left[\frac{1}{12}(1-A_0^g)+\Gamma_1-4\Gamma_2\right],\quad \frac{dt}{d\xi}=-\frac{\epsilon}{2}t+t^2\left[8-\frac{15}{2}\frac{z+\Gamma_2}{\Gamma_2}\ln\left(\frac{z+\Gamma_2}{z}\right)+\frac{1}{3}\frac{1-A_0^g}{z-1+A_0^g}\ln\left(\frac{1-A_0^g}{z}\right)\right]. \tag{1}$$

These equations are obtained after integrating fluctuations between Λ and $\lambda\Lambda$ where $\xi=-\ln\lambda^2$. The effect of the long-range part of the Coulomb interactions has been included in the above. The renormalizations of the intervalley scattering times leads to the equations

$$\frac{d\ln(1/\tau_1)}{d\xi}=t+8t\ln\left[\frac{z+\Gamma_2}{z}\right],$$
$$\frac{d\ln(1/\tau_2)}{d\xi}=\frac{15}{2}t\ln\left[\frac{z+\Gamma_2}{z}\right]+\frac{1}{2}t\ln\left[\frac{1-A_0^g}{z}\right]. \tag{2}$$

These are equations for the *physical* relaxation rates (see Ref. 7 for a discussion of this point for a related problem).

The scaling equations (1) display a metal-insulator transition very similar in nature to that discussed in Ref. 15 for the single-valley case. The transition is due to a critical *line* in the $(\Gamma_2/z,t)$ plane. Of interest in this paper is the temperature dependence of the relaxation rate $1/\tau_2$ near the critical line. This may be calculated by integrating Eqs. (1) and (2) from an initial state close to but on the metallic side of the critical line, to a final state determined by the temperature. Such a procedure yields that $1/\tau_2$ increases rapidly with temperature before saturating at a large finite value,

$$1/\tau_2(T)\approx(1/\tau_2)\exp\{15(2t_0/\epsilon)[1-(T\tau)^{\epsilon/(2+15\epsilon)}]\},$$

where t_0 is the initial value of t. However, $1/\tau_2$ cannot become larger than $kT/\hbar$ because then the scaling equations break down and the valley fluctuations are suppressed. Far from the critical line on the metallic side, I may use perturbation theory and obtain in three dimensions

$$1/\tau_2(T)=(1/\tau_2)[1+3\sqrt{3}\,|A_0^g|\,(1-1.83\sqrt{T\tau})/(E_F\tau)^2].$$

I now turn to a discussion of the interaction between the electrons and the ultrasonic phonons. The coupling of elastic strains to the electrons can be described by the following Hamiltonian as written down by Herring[16]:

$$H_{e\text{-ph}}=\frac{1}{V}\sum_{i,\alpha,\beta,\sigma}\sum_{\mathbf{k},\mathbf{p}}\int d\mathbf{r}(\Xi_d\delta_{\alpha\beta}+\Xi_u a_\alpha^i a_\beta^i)u_{\alpha\beta}(\mathbf{r})c_{\mathbf{k}i\sigma}^\dagger c_{\mathbf{p}i\sigma}e^{i(\mathbf{k}-\mathbf{p})\cdot\mathbf{r}},$$

where $u_{\alpha\beta}$ is the strain tensor, a_α^i is the α component of a unit vector directed towards the valley i, and Ξ_d and Ξ_u are the deformation-potential constants. It is now straightforward to calculate the ultrasonic phonon self-energy Π due to the electron-phonon coupling. Consider, for example, the self-energy of a longitudinal wave along the [100] direction

$$\Pi(\mathbf{q},\omega)=\frac{8}{3}\frac{\Xi_u^2\mathbf{q}^2}{\rho\omega^2}N_1(1-A_0^g)\frac{D'\mathbf{q}^2+6/\tau_2(T)}{D'\mathbf{q}^2+6/\tau_2(T)-i\omega(1-A_0^g)}, \tag{3}$$

where ρ is the mass density of the silicon lattice. The contribution above comes from the valley fluctuations associated with the Γ_c interaction. There is also an additional contribution from the number density fluctuation mode but the long-range Coulomb force suppresses it by the very small factor $\mathbf{q}^2/K^2$. (K is the inverse screening length.) Using Eq. (3), we find that the change in the velocity, c, of the longitudinal phonon along [100] is $\Delta c=-4\Xi_u^2N_1(1-A_0^g)/(3\rho c)$. This quantity is temperature independent and does not display any unusual behavior. The attenuation of the same phonon is given by the imaginary part of Π,

$$\alpha(\omega)=\frac{8\Xi_u^2}{3\rho c^3}N_1(1-A_0^g)^2\frac{\omega^2[\tau_2(T)/6]}{1+(1-A_0^g)^2\omega^2[\tau_2(T)/6]^2},$$

where the $D\mathbf{q}^2$ term has been omitted because it is very small under most experimental conditions. We note that the attenuation displays the temperature dependence of $\tau_2(T)$ which has been calculated above. Measurement of the attenuation should therefore yield useful information about the effects of diffusive valley fluctuations.

By calculating the phonon self-energy for other polarizations and directions it is easy to show that only the normal modes whose velocity depends upon the elastic constant $(c_{11}-c_{12})/2$ are affected by the coupling to the electrons.[10] The modes associated with the bulk modulus $(c_{11}+2c_{12})/3$ and c_{44} are not affected. In germanium, on the other hand, the different orientation of the valleys causes only the modes associated with c_{44} to be affected.

I conclude this paper with a summary and a discussion of the experimental conditions. Ultrasound is attenuated in doped many-valley semiconductors by processes involving the transfer of electrons between the conduction-band valleys. The attenuation is proportional to a valley relaxation time. The interaction of diffusive valley fluctuations leads to a temperature dependence of the valley relaxation time and consequently also of the ultrasonic attenuation under the following conditions: (i) The electron inelastic scattering time is long enough to satisfy $\tau_{\text{inel}}^{-1} \ll kT/\hbar$, and (ii) the temperature $(kT/\hbar)$ is larger than the valley relaxation rates $(\tau_1^{-1}, \tau_2^{-1})$. For the approximation of electrons moving in independent valleys to be valid, it is necessary that the Fermi energy be much greater than the "valley-orbit" splitting[17] of isolated donor atoms. This constrains the doping density to be considerably above the metal-insulator transition density. The independent valley picture gives a good description of the temperature dependence of the conductivity at these densities.[18] Existing measurements[19] of the ultrasonic attenuation in germanium at these densities have not gone to the low temperatures necessary to observe the effects discussed.

I would like to thank M. A. Paalanen and R. N. Bhatt for useful discussions.

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