RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 27, NUMBER 4 15 FEBRUARY 1983

# Polaron effective mass in GaAs heterostructure

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(Received 25 October 1982; revised manuscript received 13 December 1982)

The effective mass of an electron in a GaAs heterostructure is calculated in the presence of electron–LO-phonon interaction within leading-order perturbation theory. In the purely two-dimensional limit and without any screening effect, the polaron mass correction is found to be enhanced by almost a factor of 3 over the three-dimensional Fröhlich result. Inclusion of screening and the subband wave-function effects decreases the mass correction appreciably, and excellent agreement with recent experimental results reporting negligible polaronic effect in GaAs heterostructure is obtained.

A number of recent experiments[1–5] report measurements of electron effective mass in GaAs heterostructures. In these systems[6] electrons are confined in a one-dimensional (1D) potential well on the GaAs side of a GaAs-$Al_xGa_{1-x}As$ interface—the quantizing potential being provided by the donors within the $Al_xGa_{1-x}As$ side which release electrons to the GaAs conduction band lying approximately half an electron volt below that of AlGaAs. The one-dimensional potential well (in the $z$ direction, taken to be the normal to the interface) quantizes electronic motion along that direction giving rise to subbands, each of which is dynamically two-dimensional (allowing free effective-mass-like electronic motion in the $xy$ plane parallel to the interface only). When only the lowest subband is occupied by electrons, the system is two-dimensional in nature. Since GaAs is weakly polar (the Fröhlich coupling constant[7] $\alpha$ being only 0.07), these two-dimensional electrons weakly couple to the LO phonons of GaAs. This electron–LO-phonon coupling is known to modify the electron effective band mass from $M$ to $M^* = M(1+\alpha/6)$ in the bulk.[7] Thus for GaAs this correction is expected to be of the order of 1% in the bulk. This bulk polaronic correction has recently been observed[4] in cyclotron resonance measurements. However, all the measurements[1–5] carried out on GaAs heterostructure find negligible ($<1\%$) polaronic correction. As a matter of fact, Lindemann *et al.* conclude[4] that the polaronic correction in the two-dimensional GaAs heterostructure is at least a factor of 3 *smaller* than the corresponding three-dimensional bulk GaAs result. This is consistent with all the other experimetal findings[1–5] that the electron effective mass in GaAs heterostructure can be completely understood invoking only the band-structure effects (in particular, the nonparabolicity correction). Polaronic correction seems to be smaller than the experimental accuracy ($<1\%$) in all these measurements.

These experimental observations are puzzling at first sight. Purely on the basis of phase-space arguments, interaction effects are expected to be comparatively stronger in two than in three dimensions. To solve this puzzle, we calculate the electron–LO-phonon interaction correction to the electronic energy dispersion relation $E(\vec{k}) = \hbar^2k^2/2M$ in a two-dimensional system where $\vec{k}$ is a two-dimensional wave vector. We neglect any nonparabolicity corrections of the band mass $M$. Using Rayleigh-Schrödinger perturbation theory, it is straightforward to calculate the correction to the energy dispersion up to $O(\alpha)$ where $\alpha$ is the dimensionless Fröhlich coupling constant[7] for the electron–LO-phonon interaction. Since $\alpha = 0.07$ for GaAs, corrections of $O(\alpha^2)$ and higher are neglected. We get, for the corrected energy $E^*(\vec{k})$,

$$E^*(\vec{k}) = E(\vec{k}) - (\alpha\hbar\omega_{LO})K(k/q_0) \quad , \tag{1}$$

where $K(x)$ is the complete elliptic integral of the first kind and $q_0 = (2M\omega_{LO}/\hbar)^{1/2}$ with $\omega_{LO}$ as the LO-phonon frequency. For $k > q_0$ (a case in which we will not be interested in this paper), the correction vanishes.

Expanding the right-hand side of Eq. (1) up to $k^4$ we get, for small $k$,

$$E^*(\vec{k}) \cong -\epsilon_0 + \frac{\hbar^2k^2}{2M^*} - \left(\frac{9\pi\alpha}{128}\right)\left(\frac{\hbar^2k^2}{2M}\right)^2\left(\frac{1}{\hbar\omega_{LO}}\right) \quad . \tag{2}$$

The zero-order energy shift $\epsilon_0$ is given by $\epsilon_0 = \pi\alpha\hbar\omega_{LO}/2$, whereas the effective mass $M^*$ is given by $M^* = M(1+\pi\alpha/8)$. The third term in Eq. (2) is the nonparabolicity introduced by the polaron effect. Comparing with the corresponding bulk results[7] $\epsilon_0 = \alpha\hbar\omega_{LO}$ and $M^* = M(1+\alpha/6)$, we con-

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clude that the polaronic corrections are actually larger (by a factor of $\pi/2$ for the binding energy $\epsilon_0$ and by a factor of $3\pi/4$ for the effective mass $M^*$) for two-dimensional electrons compared with the three-dimensional system. This is consistent with our intuitive expectation, but is in total contradiction with experimental results[1–5] which report polaronic corrections in two-dimensional systems to be smaller than that given in Eq. (1) by an order of magnitude.

To understand this difference between the experimental results and the simple theory, we now include two physical effects that have been left out of the theory. These are (1) the screening effect and (2) the wave-function effect. Experimental conditions in Refs. 1–5 were such that free carriers of the order of $3\times10^{11}$ cm$^{-2}$ were always present during the effective-mass measurement. The presence of these free carriers affects the problem in two important ways. Firstly, screening becomes an important ingredient of the physics. Secondly, the situation cannot be taken to be just *one* electron interacting with the lattice anymore; Fermi-surface effects due to finite electron density has to be taken into account. It turns out that for the electron density $N_S(\lesssim 4\times10^{11}$ cm$^{-2}$) involved in these systems,[1–5] $k_F=(2\pi N_S)^{1/2}$ is smaller than $q_0$ and Fermi-surface effects are not so important. However, screening (which in two-dimensional systems is *independent* of $N_S$ in the simple Thomas-Fermi theory) must be taken into account. The other effect that must be included in the model is the subband wave-function effect. In the purely two-dimensional case we take the electron wave function to be of the form (neglecting normalization) $\psi(\vec{r}_{\parallel},z)=e^{i\vec{k}\cdot\vec{r}_{\parallel}}\xi(z)$ with $|\xi(z)|^2=\delta(z)$. Thus electrons are considered to be confined in an infinitesimally narrow layer. This is an idealization and, in reality, electron wave function will have some natural width $z_0$. The result of Eq. (1) is valid only in the limit of $z_0=0$. To model the actual electron wave function $\xi(z)$, we use a variational approximation[8] assuming the potential barrier at the interface to be rather large so that $\xi(z)$ can be taken to be zero for $z\lesssim0$ (we take $z=0$ plane to be the interface with the electrons confined to the $z>0$ GaAs side of the heterojunction). A suitable variational wave function for the ground state of this system is

$$\xi(z)=\left(\frac{b^3}{2}\right)^{1/2} z e^{-bz/2} , \qquad (3)$$

where $b=3/z_0$ is the variational parameter. We will not discuss the variational solution[6,8] in this paper. We just mention that the parameter $b$ and the ground-state energy $E_0$ are known[6,8] analytic functions of the electron densities and the effective mass of the system. The main effect of the wave function is to reduce the effective interaction between the confined electrons and the LO phonons.

In our calculation we use the above variational model for the wave function and employ a static Thomas-Fermi model for the screening. We get the following for the polaronic energy shift $\epsilon_0$ and the effective mass $M^*$ of the system in the presence of these two effects:

$$\epsilon_0=\frac{\pi\alpha\hbar\omega_{\rm LO}}{2}I_0 , \qquad (4)$$

and

$$M^*=M\left(1+\frac{\pi\alpha}{8}I_2\right) , \qquad (5)$$

where

$$I_0=\frac{1}{4\pi}\int_0^\infty dx\,\frac{x(8\beta^3+9\beta^2x+3\beta x^2)}{(1+x^2)(x+\gamma)(x+\beta)^3} , \qquad (6)$$

and

$$I_2=\frac{2}{\pi}\int_0^\infty dx\,\frac{x^3(8\beta^3+9\beta^2x+3\beta x^2)}{(1+x^2)^3(x+\gamma)(x+\beta)^3} . \qquad (7)$$

The parameters $\gamma$ and $\beta$ are given by $\gamma=q_{\rm TF}/q_0$ and $\beta=b/q_0$. The two-dimensional screening constant $q_{\rm TF}$ is obtained within the simple long-wavelength Thomas-Fermi theory,[9] $q_{\rm TF}=2Me^2/\kappa\hbar^2$ with $\kappa$ the lattice dielectric constant of GaAs.

The integrals $I_0$ and $I_2$ are obtained numerically for a variety of values of the parameters $\gamma$ and $\beta$. We note that we recover the purely two-dimensional, unscreened result if we take $\gamma=0$ and $\beta=\infty$ limit of Eqs. (6) and (7). We present our results in terms of the known three-dimensional results by writing $\epsilon_r=\epsilon_0^{\rm 2D}/\epsilon_0^{\rm 3D}=(\pi/2)I_0$ and $\Delta M_r=\Delta M_{\rm 2D}/\Delta M_{\rm 3D}=(3\pi/4)I_2$ where we clearly understand that the three-dimensional results have been obtained with only one electron interacting with the polar lattice (i.e., *without* any screening). We define $\Delta M=(M^*-M)/M$.

In Fig. 1 we show $\epsilon_r$ as a function of $\beta$ for a number of values of $\gamma$. For $\beta$ very large and $\gamma$ very small, we recover the expected two-dimensional result $\epsilon_r=\pi/2$. However, depending on the actual values of $\gamma$ and $\beta$, $\epsilon_r$ could be much smaller than unity, as has been seen experimentally. For example, the experimental conditions of Ref. 4 correspond to $\gamma,\beta\simeq1$ whence we find that $\epsilon_r=0.18$ which is almost a factor of 10 smaller than the purely two-dimensional result. In Fig. 2 we show $\Delta M_r$ as a function of $\beta$ for a number of values of $\gamma$. Again the two-dimensional result is recovered for large $\beta$ (i.e., small $z_0=3/b$) and small $\gamma$ (i.e., small $q_{\rm TF}$). For the experimental situation of Ref. 4, we get $\Delta M_r=0.34$, which is about a factor of 7 smaller than the purely two-dimensional result.

For any particular situation we can obtain $\epsilon_r$ and $\Delta M_r$ from Figs. 1 and 2 by using the expressions for $q_0$ and $q_{\rm TF}$ given earlier in the paper and by using the variational[6] result $b=(48\pi MNe^2/\kappa\hbar^2)^{1/3}$, where $N=N_d+(11/32)N_s$ and $N_d$ and $N_s$ are the depletion and the carrier densities, respectively. For GaAs, taking $N=10^{11}$ cm$^{-2}$, we get $q_0=2.6\times10^6$ cm$^{-1}$,

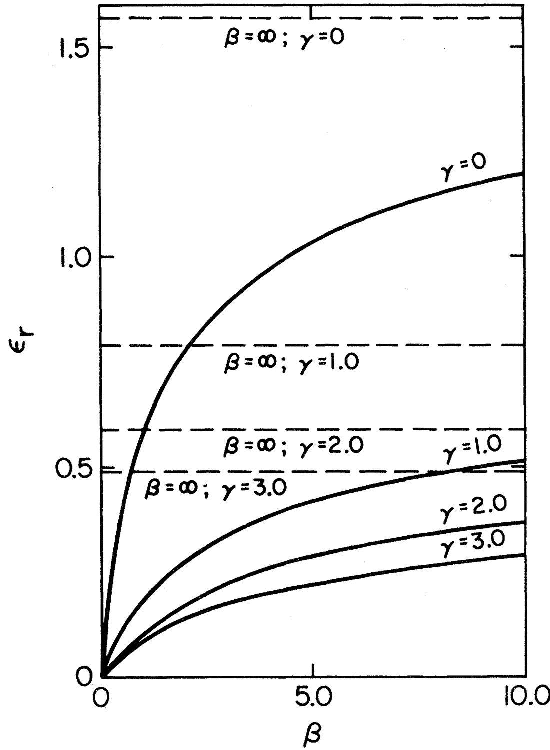


FIG. 1. Shows the polaron binding energy $\epsilon_r = \epsilon_0^{2D}/\epsilon_0^{3D}$ in the two-dimensional heterostructures in the units of the corresponding bulk result $\epsilon_0^{3D} = \alpha\hbar\omega_{LO}$, as a function of the wave-function parameter $\beta = b/q_0$ for four values of the screening parameter $\gamma = q_{TF}/q_0 = 0$, 1.0, 2.0, and 3.0. For each of the curves the limiting pure two-dimensional ($\beta = \infty$) result is shown by the dashed line.

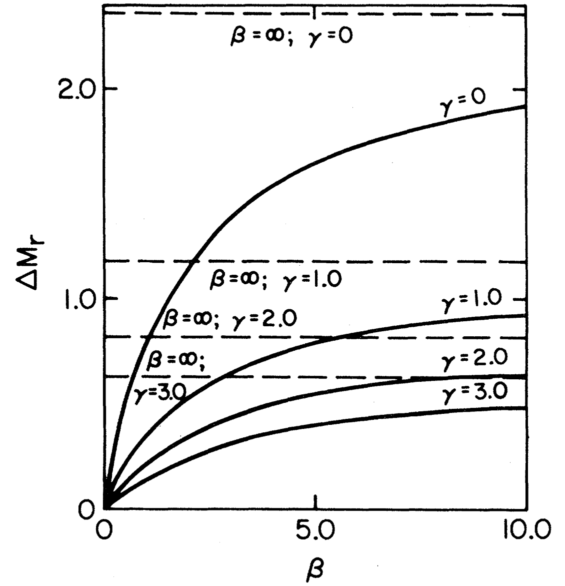


FIG. 2. Shows the polaron mass correction $\Delta M_r = \Delta M_{2D}/\Delta M_{3D}$ in the two-dimensional heterostructure, in the units of the corresponding bulk result $\Delta M_{3D} = \alpha/6$, as a function of the parameter $\beta = b/q_0$ for four values of the parameter $\gamma = q_{TF}/q_0$. The mass correction is defined by $\Delta M = (M^* - M)/M$ and the dashed lines indicate the purely two-dimensional limits ($\beta = \infty$) for each curve.

$q_{TF} = 2.2 \times 10^6$ cm$^{-1}$, and $b = 2.6 \times 10^6$ cm$^{-1}$. This corresponds to $\gamma = 0.85$ and $\beta = 1.0$, giving $\Delta M_r = 0.4$. The important point we want to emphasize here is that the polaronic effective-mass correction in GaAs heterostructure is indeed rather small when all the effects are taken into account. This is in excellent agreement with experimental observations.[1–5] This clearly shows the importance of including the screening and the subband wave-function effects in the calculation of polaronic corrections. It will be misleading to state that polaronic effects are smaller in two dimensions compared with the three-dimensional case. As we have shown explicitly in this paper, the purely two-dimensional result is actually enhanced over the three-dimensional value; however, the screening and the wave-function effects reduce the effective polaronic correction in GaAs heterostructure by almost an order of magnitude giving excellent agreement with the null experimental results.[1–5]

In conclusion, we calculate the electron effective mass in the GaAs heterostructure in the presence of electron–LO-phonon interaction, taking into account electronic screening and subband wave-function effects. We find that in the purely two-dimensional no screening limit polaron corrections are appreciable. But, inclusion of the screening and the subband effects reduce the polaron effects considerably, giving good agreement with experimental observations. To observe enhanced polaronic effect in a two-dimensional system we suggest experiments in heterostructures without containing many free carriers. This can be done by photoexciting carriers in GaAs heterostructure or probably more conveniently by doing an experiment in nipi system.[10] To reduce the wave-function effect, one should probably do the experiment on rather thin layers of GaAs. Also, materials with higher values of the Fröhlich constant ($\alpha$) may be more suitable for observing the two-dimensional enhancement discussed in this paper. One such material[11] could be inversion or accumulation layers on HgCdTe.

## ACKNOWLEDGMENTS

The author acknowledges helpful discussions with G. Abstreiter, A. B. Fowler, E. Gornik, and F. Koch. He also thanks V. Korenman for a critical reading of the manuscript. The author is grateful to the University of Maryland Computer Center for providing the computer time needed in this work. The work is supported in part by the National Science Foundation through Grant No. NSF-DMR 79908810.

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