“Universal” Conduction-Band Structure in Some Common Semiconductor Compounds

E. A. Johnson,⁽¹⁾ A. MacKinnon,⁽¹⁾ E. P. O'Reilly,⁽²⁾ and M. Silver⁽²⁾

⁽¹⁾*Blackett Laboratory, Imperial College, London SW7 2BZ, United Kingdom*

⁽²⁾*Department of Physics, University of Surrey, Guildford, Surrey GU2 5XH, United Kingdom*

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The conduction bands of direct-gap III-V semiconductors are shown to be effectively universal near the Γ point even when strongly nonparabolic, for energies in effective rydbergs and wave numbers in inverse effective lattice constants. This implies universality of the diamagnetic Shubnikov-de Haas effect in the nonparabolic regime in some two-dimensional electron gases, as observed experimentally. A two-band $\mathbf{k} \cdot \mathbf{p}$ approximation together with Harrison's model-solid theory explains this near universality and relates its systematic small deviations to the covalency of the material in question.

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It was first pointed out by Zhao *et al.*¹ that universal behavior seemed to hold for the diamagnetic shift observed in the subbands of some two-dimensional electron systems in the presence of a transverse magnetic field (the diamagnetic Shubnikov-de Haas effect). It was observed by these authors that the cutoff magnetic fields at which various subbands became depleted apparently fell on common curves when plotted against the strength of the potential well, provided that field strength and well strength were properly scaled, irrespective of the semiconductor material involved. This apparent universality has been observed both in spike- (δ -) doped quantum wells²⁻⁴ and in heterojunctions and charge-accumulation layers,^{1,5-7} and is apparently unaffected by nonparabolicity in the band structure of the host materials, even for energies where such nonparabolicity should be important.

As pointed out by Reisinger and Koch,² this universality is a consequence of the scaling property of the simple effective-mass equation for the envelope function, as in the theory of shallow donors.⁸ These authors² also present (universal) predictions for the diamagnetic Shubnikov-de Haas effect, calculated self-consistently in the parabolic-band approximation, which agree well with experiment when nonparabolic effects can be neglected. What is surprising, however, is the persistence of an observed universality in circumstances where nonparabolicity should be important, and in which some deviation from the Reisinger and Koch² predictions is apparent.⁷

It is the purpose of the present work to show how the observed universality can hold even when the band structure of the host semiconductor is strongly nonparabolic. In the process, we clarify the conditions under which this might happen, and emphasize the variety of consequences which follow from the scaling property of the effective-mass theorem as applied to simple Coulomb systems.

The simple effective-mass equation may be written

$$\left[\frac{-\hbar^2}{2m^*} \nabla^2 + V(\mathbf{r}) \right] \psi(\mathbf{r}) = E\psi(\mathbf{r}), \quad (1)$$

where $\psi(\mathbf{r})$ is the envelope function, $V(\mathbf{r})$ the externally imposed potential, and m^* the ($\mathbf{k}=0$) effective mass. For electronic structure calculations in δ wells or accumulation layers, $V(\mathbf{r})$ is commonly taken to be an idealized potential (that of a uniformly charged plane layer for the δ well, and a sharp band-edge discontinuity for an accumulation layer). We work within this approximation here, thus assuming that system nonuniformities may be neglected in the first instance. The use of Eq. (1) also implies that phenomena on the scale of a lattice constant are effectively averaged out in the regime considered (thus, e.g., that central-cell corrections are negligible). This approximation is even more easily justified since calculations indicate that even for strong confinement the extent of the wave function is large on the scale of a lattice constant.

In the theory of shallow donors,⁸

$$V(\mathbf{r}) = -e^2/\epsilon r, \quad (2)$$

in Eq. (1), where ϵ is the static dielectric constant. The effective-mass equation (1) for this case has the property that its material-dependent parameters, m^* and ϵ , can be removed by scaling all distances r in terms of the effective Bohr radius $a^* = \hbar^2 \epsilon / m^* e^2$, with energies then automatically scaled in effective rydbergs, $\text{Ry}^* = e^2 / 2\epsilon a^*$. Scaled thus, the properties of shallow donors are independent of the properties of the host semiconductor, and therefore universal. This universality persists when self-consistent effects are taken into account, since the self-consistent corrections to Eq. (2) are simple Coulomb effects proportional to e^2/ϵ , and therefore scale in the same way as the original ion potential (2).

This scaling property holds for other simple Coulomb systems, as was suggested by Reisinger and Koch,² even in the presence of an external magnetic field. It is evident from the foregoing, however, that for this to be true, the external potential must be one which does not introduce any new length or energy scale into the effective-mass equation (1) (note that an external magnetic field introduces no *new* length scale). An ideal δ well is such a simple Coulomb system; a heterojunction

approximates such a system only if it is well described by a band edge with an infinite potential step.

It follows that if one has a simple Coulomb system, then it should show universal behavior in every respect, in the regimes considered here. Thus, any property (e.g., subband energies, wave functions, or subband fillings) should be independent of the host semiconductor material when measured in the correct units, the universal diamagnetic Shubnikov-de Haas effect being only one of a class of observable universalities.

The effective-mass equation (1) is only correct for materials with a parabolic-band structure. More generally, the effective-mass theorem states that

$$[E(-i\nabla) + V(\mathbf{r})]\psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (3)$$

for a material with known but unspecified band structure $E(\mathbf{k})$. Experiment indicates that universality can persist in simple Coulomb systems even when $E(\mathbf{k})$ is strongly nonparabolic. We note, however, that all of the universal scaling consequences of Eq. (1) would persist if it should happen that *the band structures of the materials in question were themselves universal*. For this to be the case, $E(\mathbf{k})$ should be the *same* function of $\mathbf{k}$, for each host semiconductor, when E is measured in Ry^* and $\mathbf{k}$ in units of $2\pi/a^*$, i.e., $E/(1 \text{ Ry}^*) = F(ka^*/2\pi)$ with F the same function for all materials, even when nonparabolicity is important.

To test this hypothesis, we begin by calculating the conduction-band structure of the five direct-gap III-V semiconductors, using the empirical pseudopotential method with the local approximation, including spin-orbit interactions. The material parameters have been taken from Cohen and Bergstresser.⁹ Energies are scaled in terms of Ry^* , and wave vectors in terms of $2\pi/a^*$. Figure 1 shows these scaled band structures along the [100] and [111] directions, along with the scaled parabolic-band structure common to all materials. The agreement in band structure among the five materials is striking, even for energies far outside the parabolic region. This is most evident in the [100] direction, but is also true along [111] for the range of k values of experimental relevance.

The generalized effective-mass equation (3) is applicable for values of $\mathbf{k}$ which are small on the scale of a Brillouin zone, say, $k \leq 0.1(2\pi/a)$, where a is the lattice constant. This limit translates into a scaled k value of 1.47 for InP, 1.74 for GaAs, 3.31 for GaSb, 5.54 for InAs, and 9.66 for InSb. Experiments in δ wells and in charge layers have remained within this small- k regime. There is thus a large range of small k in most of these materials over which the band structure is *strongly nonparabolic* but also *approximately universal*.

To quantify this, consider a reduced k of 1.5 in Fig. 1 (just over 0.1 of a zone, with $E \sim 450 \text{ meV}$, for InP). Along [100] the band structures agree to within a relative standard deviation $\sigma = 0.015$, while the deviation from parabolic is 20σ . The influence of subsidiary mini-

FIG. 1. Conduction-band structures for the direct-gap III-V semiconductors, from empirical pseudopotential calculations, plotted along the [111] and [100] directions (left-hand side and right-hand side of the figure, respectively); energy in effective rydbergs, wave number in units of $2\pi/a^*$.

ma gives worse agreement along [111], but even there the predicted band structures agree within a σ of 0.052.

A $\mathbf{k} \cdot \mathbf{p}$ calculation gives similar results. In the full Kane¹⁰ three-level model, the conduction-band dispersion is obtained from the interaction between the conduction band and the three nearest (light-hole, heavy-hole, and spin-split-off) valence bands. One obtains

$$E'(E' + E_G)(E' + E_G + E_{SSO}) - k^2 P^2 (E' + E_G + \frac{2}{3} E_{SSO}) = 0 \quad (4)$$

for the relation between the electron's energy

$$E = E' + \hbar^2 k^2 / 2m_e \quad (5)$$

and its wave number k . Here E_G is the $k=0$ energy gap between valence and conduction bands, E_{SSO} is the gap between valence and spin-split-off bands, and m_e is the free-electron mass. In Eq. (4) the energy zero is at the bottom of the conduction band; the Kane¹⁰ matrix element P has been fitted to the experimental $k=0$ effective mass of each material. The results are shown in Fig. 2(a), which also includes the II-VI material $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$, for comparison. Again, there is close agreement among the predicted conduction-band structures and a wide deviation from the similarly scaled parabolic-band structure.

More insight into this phenomenon can be obtained by replacing Eq. (4) by a quadratic two-band approximation, in which the band parameters E_G and E_{SSO} are replaced by a single effective band gap

$$E_{\text{eff}} = E_G(E_G + E_{SSO}) / (E_G + \frac{2}{3} E_{SSO}),$$

chosen so that the conduction-band effective mass is that

FIG. 2. (a) Conduction-band dispersion as in Fig. 1, from the Kane three-level approximation (curves for GaAs and InAs nearly coincide). The II-VI material $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$ is also included. Each curve is valid in the small- k limit described in the text. (b) As in (a), from the two-band approximation described in the text. These band structures are very close to the corresponding curves in (a), thus confirming the usefulness of the two-band model.

of Eq. (4). The resultant two-band model reproduces very effectively the three-level scaled conduction-band structure, as shown in Fig. 2(b) [here the parameter P is chosen as in Fig. 2(a)].

In the two-band approximation, Eq. (4) is replaced by

$$E'(E' + E_{\text{eff}}) - k^2 P^2 = 0. \quad (6)$$

Neglecting the free-electron correction (5), E_{eff} can be eliminated using the relation $m^* = \hbar^2 E_{\text{eff}} / 2P^2$ to give

$$\hbar^2 E / P^2 m^* = [1 + (\hbar^2 k / P m^*)^2]^{1/2} - 1. \quad (7)$$

This relation is *exactly* universal in the scaled variables $E/P^2 m^*$ and $k/P m^*$. In the reduced variables $E_r = E/(1 \text{ Ry}^*)$, $k_r = \hbar k a^*/2\pi$ considered here, however, Eq. (7) becomes

$$k_r = \left[\frac{1}{2\pi} \right]^2 \left[E_r + \frac{e^4}{4} \frac{1}{\epsilon^2 P^2} E_r^2 \right]^{1/2}; \quad (8)$$

TABLE I. Kane matrix element P (in eV Å), static dielectric constant ϵ , product ϵP , covalency α_c , and ratio $\epsilon P / \alpha_c^3$ for the direct-gap III-V semiconductor compounds.

	P_{exp}^a	ϵ^a	ϵP	α_c^b	$\epsilon P / \alpha_c^3$
GaSb	9.24–10.14	15.69 ± 0.85^c	137–168	0.89	194–238
GaAs	9.66–9.90	12.2–13.6	118–135	0.88	173–198
InSb	9.41 ± 0.11^c	16.6–18.0	154–172	0.85	251–280
InAs	8.51–9.20	15.15 ± 0.82^c	122–147	0.83	213–257
InP	7.98–8.82	11.73–12.61	94–111	0.81	176–209

^aLandolt-Börnstein Numerical Data and Functional Relationships in Science and Technology, edited by O. Madelung (Springer-Verlag, New York, 1982), Group 3, Vol. 17, Pt. a; *ibid.*, Vol. 22, Pt. a.

^b α_c from Eq. (9) and Ref. 11, Table 4-1.

^cUncertainty estimated from that in GaAs.

a relation which would only be universal if ϵP were constant. The effective universality of III-V conduction-band structures follows from the fact that, as shown in Table I, ϵP indeed has very similar values for these compounds.

Further understanding of the role of the factor ϵP in effective universality comes from the semiquantitative band-structure calculations described by Harrison.¹¹ In that approach, P is shown to depend upon material¹² through the nearest-neighbor bond length d , as $P \propto d^{-1}$, while for the static susceptibility χ one obtains¹³

$$\epsilon = 1 + 4\pi\chi \approx 4\pi\chi, \quad \chi \propto \alpha_c^3 d, \quad (9)$$

where $\alpha_c = V_2/(V_2^2 + V_3^2)^{1/2}$ is the covalency of the material (V_2 is the covalent and V_3 the polar energy¹⁴). Thus, approximately,

$$\epsilon P \propto \alpha_c^3. \quad (10)$$

Table I (final column) shows that relation (10) agrees at least qualitatively with experiment. The approximate constancy of ϵP thus follows from that of the covalency α_c of the III-V semiconductor compounds.

Equations (7) and (10) predict that approximate universality should be a general property of semiconductors.¹⁵ They also predict that deviations from universality are related to the covalency α_c , with nonparabolicity increasing as α_c decreases. The entries in Table I are ordered by decreasing values of α_c . Comparison with Figs. 1 and 2 shows that the calculated band structures tend to follow this ordering. Equation (10) also suggests that II-VI band structures should be more nonparabolic than III-V's, when plotted in reduced variables; this is confirmed for $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$ in Fig. 2(a).

In conclusion, an observed universality in the diamagnetic Shubnikov-de Haas behavior of some simple Coulomb systems (in δ wells and approximately in heterojunctions) is explained by an effectively universal $E(\mathbf{k})$ conduction-band relation near the Γ point in common semiconductor materials, in a regime where narrower-gap materials show strong deviations from par-

abolicity. This result implies that all other aspects of the small- k conduction-band electronic structure of these systems should also be approximately universal in the same materials. Deviations from universality are shown to be small and to depend upon covalency of the material in question. An explanation of both these facts is obtained from a two-band approximation (6) together with approximate electronic structure predictions following from Harrison.¹¹

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¹⁴Equations (4-18) and (4-19) in Ref. 11.

¹⁵Thus, e.g., universality should be an even better approximation for the Γ -point conduction-band structures of the group-IV semiconductors than it is for the III-V's.