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Solid-state analogue of the relativistic gases

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An exact analogy is developed here between particles in a nonparabolic band of a semiconductor (nonparabolicity parameter $E_0 \sim \frac{1}{2}E_G$, energy gap E_G) and a gas of particles of rest mass m_0 moving with relativistic velocities. The connection is made by replacing the velocity of light in the relativistic theory by the velocity $v=(E_0/m_0^*)^{1/2}$, where m_0^* is the effective mass at the band extremum. For InSb (conduction band), $v \sim 1.1\times10^8$ cm/s. The rest energy $\varepsilon_0 \equiv m_0c^2$ of the relativistic theory is then replaced by $E_0 \equiv m_0^* v^2$. A compressive stress, for example, which increases nonparabolicity corresponds to a gas which is rendered more relativistic because E_0 has been decreased relative to kT. The density of states corresponding to the dispersion relation $\hbar^2k^2/2m_0^* = E(1+E/2E_0)$ is shown to be of the same form as that for an ideal special relativistic gas. The well-known relativistic change of mass with velocity is also reproduced exactly in the solid-state case, and not only approximately as hitherto supposed. The thermodynamic quantities such as the mean number of particles, the mean energy, and the pressure of the gas are all given in terms of modified Bessel functions K_ν of the argument kT/E_0.

I. INTRODUCTION

It is pointed out in this paper for the first time that the analogy between particles in a conduction band with a nonparabolicity parameter E_0 (an energy) and a gas of particles of rest mass m_0 which move with relativistic velocities is exact and not approximate as hitherto supposed. On approaching the limit of a parabolic band, E_0 increases to infinity and this corresponds to a relativistic gas of particles which are sufficiently heavy to behave nonrelativistically. If E_0 is small compared with kT, however, the corresponding gas can be treated in the extreme relativistic limit. This suggests new physical ways of looking at solid-state experiments using

$$E_0 \equiv m_0^* v^2, \quad E_0 \sim E_G/2 , \tag{1}$$

where m_0^* is the effective mass at the band extremum and the velocity v and the energy E_0 are related by (1). The analogy is then simply obtained by replacing the velocity of light of the relativistic theory by v, and the rest mass by m_0^*:

$$\begin{aligned} &\varepsilon_0 \equiv m_0c^2 \leftrightarrow E_0 \equiv m_0^* v^2 \simeq \tfrac{1}{2}E_G , \\ &(m_0, c) \leftrightarrow (m_0^*, v) . \end{aligned} \tag{2}$$

For the conduction band of InSb, $m_0^* \sim 0.013 m_0^*$, $E_G \sim 0.18$ eV so that, interpreting $2E_0$ as E_G^{-1}, one finds $v \sim 1.1\times10^8$ cm/s, which is 0.37% of the velocity of light. Thus some relativistic type experiments can be performed more readily in the solid state because $v \ll c$. This has been noted before;[1,2] it is, however, the exactness of the analogy which occupies us here. The systems considered here stand between the nonrelativistic gases ($\varepsilon_0 \rightarrow \infty$) and the extreme relativistic gases ($\varepsilon \rightarrow 0$).

The analogy between the forbidden gap in a semiconductor and the energy $2m_0c^2$ needed for the creation of particle-antiparticle pairs has occasionally been noted. Also, the two-band effective mass theory has been related to the Dirac equation.[3] But this is quite different from the exact analogy discussed here, which covers the density of states and the change of mass with velocity.

The analogy applies most simply to the conduction band of semiconductors of energy gap E_G which can be described by a dispersion relation of the Kane-type[4]

$$\frac{\hbar^2k^2}{2m_0^*} = \frac{(3E_G+2\Delta)(E+E_G)(E+E_G+\Delta)}{3E_G(E_G+\Delta)(E_G+E+\frac{2}{3}\Delta)}E , \tag{3}$$

where E is the carrier kinetic energy above the bottom of the band and Δ is the spin-orbit splitting of the valence band. The relation (3) can often be approximated by

$$\frac{p^2}{2m_0^*} = \frac{\hbar^2k^2}{2m_0^*} = E\left[1+\frac{E}{2E_0}\right] . \tag{4}$$

The simplified form (4) certainly applies if $\Delta \rightarrow 0$ or $\Delta \rightarrow \infty$. In other cases one can show that for all Δ and E

$$1 \ge \frac{\hbar^2k^2}{2m_0^*}\frac{1}{E(1+E/E_G)} \ge \frac{2}{3} . \tag{5}$$

For our purposes it is adequate to treat E_0 in Eq. (4) simply as a parameter and to use (4) rather than (3).

II. SOME PAST USES OF THE DISPERSION RELATION (4)

The two-band Kane model as expressed by Eq. (4) is widely used for the conduction bands of semiconductors, particularly the III-V compounds. As no review article of such studies seems to be available, we merely cite some relevant recent work. In silicon the piezo-resistance was studied in this way recently;[5] in InSb the metal-insulator semiconductor capacitance,[6] surface waves,[7] and the heat

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capacity of thin films[8] could be discussed with the aid of the dispersion relation (4); it was used for gallium arsenide to study the Boltzmann equation for the interaction of energetic electrons with polar optical phonons.[9] Note also studies of nonparabolicity by the measurement of thermoelectric power in a strong magnetic field, applied for example to lead compounds[10] and the inclusion of the effect of nonparabolicity in the study of the hot electron distribution in InSb.[11] We shall apply the new interpretation to the first of these references.[5] This examines the stress dependence of the resistivity of the conduction band of n-type silicon. Application of a compressive stress makes the electron gas more relativistic, or the "rest energy" E_0 smaller with respect to kT. This is equivalent to speaking about increased nonparabolicity or alternatively about a greater departure from the nonrelativistic limit. The effect of the dispersion relation (4) on the activity coefficient and the Einstein mobility-diffusion coefficient ratio, and the equation which connects them, has recently been investigated in a companion paper.[12] The electron behavior in InSb in crossed magnetic and electric fields has been considered experimentally and theoretically in a paper issued since the work on this paper and on Ref. 12 was completed.[2] There the analogy expressed by Eq. (2) was noted independently. The present considerations may suggest further developments of this work. For example, the rise in effective mass at the Fermi level with electron concentration is due to nonparabolicity and corresponds to the relativistic rise of mass with velocity.[1,13] But this analogy was believed to depend on the approximation $|E/E_0| \ll 1$. Because of band curvature, effective mass increase with electron concentration is in any case expected as a general feature. This applies to the average mass or the mass at the Fermi level. See Ref. 14 for the case of the silicon optical effective mass.

III. THE ANALOGY FOR THE DENSITY OF STATES AND ITS CONSEQUENCES

In this section we note the *exact* analogy for the density of states. For spin degeneracy g and volume V the density of states implied by (4) is, in virtue of

$$(gV/2\pi^2)k^2 dk/dE \ , \tag{6}$$

given by

$$N(E)=\frac{4\pi gV}{h^3v^3}(E+E_0)(E^2+2E_0E)^{1/2} \ . \tag{7}$$

This is precisely the density of states for a gas of particles moving with relativistic velocities,[15] except that the velocity of light is here replaced by the velocity v defined in (1). In the simplest case $(E_0 \sim E_G/2)$, we have $v \sim (E_G/2m_0^*)^{1/2}$, and this quantity can be treated as a constant as far as integrations over the kinetic energy E are concerned. Note $N(E) \propto E^{1/2}$ (as $E_0 \rightarrow \infty$), and $N(E) \propto E^2$ (as $E_0 \rightarrow 0$), which are characteristic energy dependencies familiar from parabolic bands and from black-body or Debye specific-heat theories, respectively.

Consider now a gas subject to (4) with a mean number N of fermions, mean kinetic energy U, pressure p, temperature T, chemical potential μ, and spin degeneracy g in a volume V. Using

$$G((E-\mu)/kT) \equiv \left[\frac{4\pi gV}{3h^3v^3}\frac{1}{\exp[(E-\mu)/kT]+1}\right] \times (E^2+2E_0E)^{1/2} \ ,$$

one finds (see Table I)

$$\left.\begin{matrix} N \\ U \\ pV \end{matrix}\right\} = \int_0^\infty G\left[\frac{E-\mu}{kT}\right] \times \begin{Bmatrix} 3(E+E_0) \\ 3E(E+E_0) \\ E(E+E_0) \end{Bmatrix} dE \ . \quad \begin{matrix} (8a) \\ (8b) \\ (8c) \end{matrix}$$

With $N_c \equiv (2\pi m_0^* kT/h^2)^{3/2} gV$, this goes over into a usual result in the parabolic limit $E_0 \rightarrow \infty$:

$$\left.\begin{matrix} N \\ U \\ pV \end{matrix}\right\} = N_c \begin{cases} I(\frac{1}{2},\mu/kT) & (9a) \\ \frac{3}{2}kT\, I(\frac{3}{2},\mu/kT) & (9b) \\ kT\, I(\frac{3}{2},\mu/kT) & (9c) \end{cases}$$

where

TABLE I. Main integrals for a relativistic ideal gas over the kinetic energy E. $B \equiv 4\pi gV/3h^3v^3$, $\beta \equiv (\mu - E_0)/kT$, μ is the chemical potential, and $\eta = \pm 1$.

Number of particles,	$N = 3B\int_0^\infty \frac{(E+E_0)(E^2+2EE_0)^{1/2}}{\exp[(E/kT)-\beta]+\eta}dE$
Internal energy U (excluding E_0)	$=3B\int_0^\infty \frac{(E^2+EE_0)(E^2+2EE_0)^{1/2}}{\exp[(E/kT)-\beta]+\eta}dE$
Pressure,	$p=\frac{B}{V}\int_0^\infty \frac{(E^2+2EE_0)^{3/2}}{\exp[(E/kT)-\beta]+\eta}dE$

$$\Gamma(s+1)I(s,\mu/kT) \equiv \int_0^\infty \{x^s/[\exp(x-\mu/kT)+1]\}dx \ .$$

In order to evaluate the integrals in (8), it is convenient to use the substitution

$$E/m_0^* v^2 + 1 = \cosh\theta \ ,$$

which leads to ($s \equiv \sinh\theta$, $c \equiv \cosh\theta$)

$$\left.\begin{matrix} N \\ U \\ pV \end{matrix}\right\} = \int_0^\infty H(\theta,\mu/kT) \times \left\{\begin{matrix} \dfrac{3}{m_0^* v^2} s^2 c & \text{(10a)} \\ 3s^2 c(c-1) & \text{(10b)} \\ s^4 & \text{(10c)} \end{matrix}\right\} d\theta \ ,$$

where

$$H(\theta,\mu/kT) \equiv \frac{4\pi g V (m_0^*)^4 v^5}{3h^3} \frac{1}{\exp[(m_0^* v^2/kT)(\cosh\theta - 1) - \mu/kT] + 1} \ . \tag{11}$$

This is very similar to the corresponding expressions for a relativistic gas,[12,15,16] except that the energy in the exponent of Eq. (11) is there the total energy, including the rest energy, and this either removes the -1 or leads to a renormalization $\mu \rightarrow \mu_r \equiv \mu - mc^2$ of the chemical potential in the relativistic case. The long history of discussions of such integrals was summarized in Ref. 17 (see also Ref. 18). Numerical work performed for the integrals in the solid-state context[19] was of course done without knowledge of this analytical work on the same integrals for the relativistic gases.

Let us put for the nondegenerate case

$$N_c \equiv \left[\frac{2\pi m_0^* kT}{h^2}\right]^{3/2} gV \ ,$$

$$X \equiv \tfrac{1}{4}[3K_3(E_0/kT) + K_1(E_0/kT)] - K_2(E_0/kT) \ .$$

The integrations in (10) may be performed by standard methods[15,18] and lead to modified Bessel functions:

$$\left.\begin{matrix} N \\ U \end{matrix}\right\} = \frac{N_c}{(\pi kT/2E_0)^{1/2}} \times \exp[1/kT(E_0+\mu)] \times \left\{\begin{matrix} K_2(E_0/kT) & \text{(12a)} \\ E_0 X \ . & \text{(12b)} \end{matrix}\right.$$

In addition, $pV = NkT$. In the limit $E_0 \rightarrow \infty$ the nondegenerate version of (9) is found; one merely has to replace $I(s,\mu/kT)$ by $\exp(\mu/kT)$.

The effect of nonparabolicity in raising the ratio U/nkT and the heat capacity C_v/Nk of a nondegenerate electron gas is shown in Fig. 1 (see also Ref. 13). The case of conduction-band electrons in InSb at room temperature is marked by an arrow. For ideal quantum gases U/NkT ranges from $\frac{3}{2}$ in the nonrelativistic limit to 3 in the extreme relativistic limit (which applies, for example, to black-body radiation or particles with zero rest mass). While the first case corresponds to the parabolic limit $E_0 \rightarrow \infty$ in the solid-state case, there is no obvious analogue which corresponds to the second limit. This requires $E_0 \rightarrow 0$, i.e., a vanishing effective mass at the band extremum.

When one goes to more complicated band structures such as the narrow gap tetragonal material Cd_3As_2, to mention just one example, the simple analogy discussed here is of course lost again because of the much more complicated density of states.[20]

The integrals in Table I can be developed in a series of modified Bessel functions $K_\nu(x)$, even for a gas in d dimensions (see, for example, Ref. 18). Approximate methods can also be used (see, for example, Ref. 21).

IV. THE CHANGE OF MASS WITH VELOCITY

From (4), using (1),

$$p^2 v^2 + E_0^2 = (E + E_0)^2 \tag{13}$$

which is an equation for E in terms of $p = \hbar k$. The Hamiltonian equation of motion

$$\dot{x}_j = \partial H(p_1, p_2, \ldots; q_1, q_2, \ldots)/\partial p_j \ ,$$

i.e., $w = dE/dp$, then yields the velocity at a general momentum value as

$$w = pv^2(p^2 v^2 + E_0^2)^{-1/2} \ . \tag{14}$$

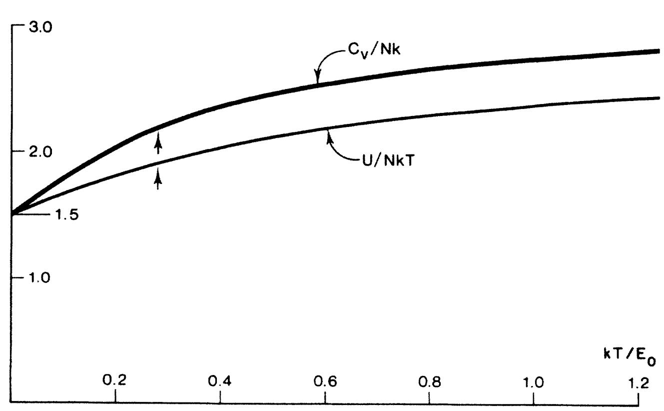

FIG. 1. The ratios U/NkT and C_v/NkT for a nondegenerate electron gas as a function of the nonparabolicity parameter. The numerical data of Table 24 of Ref. 15 have been used.

This is the velocity one would find from the more familiar solid-state formula $\mathbf{w}=\hbar^{-1}\mathrm{grad}_{\mathbf{k}}E(\mathbf{k})$. But the formulation in terms of the momentum $p=\hbar k$ is also applicable to the relativistic situation using the replacement (2). One finds

$$\frac{w^2}{v^2}=\frac{p^2v^2}{p^2v^2+E_0^2}=\frac{E^2+2EE_0}{(E+E_0)^2} \tag{15}$$

which shows at once that v of (2) can also be introduced as the limiting velocity which is reached for large E.

In the solid state one uses two distinct masses: the "momentum" mass $\tilde{m}$ which enters into cyclotron-resonance experiments, and the "acceleration" mass m^*. The former is defined by

$$\tilde{m}^2\equiv\left[\frac{p}{w}\right]^2=\frac{p^2v^2+E_0^2}{v^4}=\left[\frac{m_0^*}{E_0}(E+E_0)\right]^2, \tag{16}$$

where (13) and (14) have been used. It follows, using (15), that

$$\frac{\tilde{m}}{m_0^*}=1+\frac{E}{E_0}=\left[1-\frac{w^2}{v^2}\right]^{-1/2}. \tag{17}$$

This is the relation required. A plot of $(\tilde{m})^{-2}$ against w^2 (measured independently) should yield a falling straight line with intercept $(m_0^*)^{-2}$ and slope $-(E_0m_0^*)^{-1}$, in which case (17) would be confirmed experimentally. The whole argument is also valid for special relativity and shows that also in this respect the solid-state analogy for a relativistic particle is exact.

The effective mass tensor for band n at wave vector $\mathbf{k}$ is in the isotropic case (the only one of interest here)

$$\left[\frac{1}{m^*}\right]_{ii}^{n,\mathbf{k}}\equiv\hbar^{-2}\frac{\partial^2E_n(\mathbf{k})}{\partial k_i^2}=\frac{\partial^2E_n(\mathbf{p})}{\partial p_i^2}.$$

It relates acceleration $\mathbf{a}$ to force $\mathbf{F}$ acting on the particle:

$$\mathbf{a}=(m^*)^{-1}\mathbf{F}. \tag{18}$$

In this isotropic case the acceleration mass may therefore be defined by

$$(m^*)^{-1}\equiv\frac{d^2E}{dp^2}=\frac{dw}{dp}=\frac{v^2E_0^2}{(E+E_0)^3}. \tag{19}$$

Using (17) and (19),

$$\frac{m^*}{m_0^*}=\left[1+\frac{E}{E_0}\right]^3=\left[1-\left[\frac{w}{v}\right]^2\right]^{-3/2}. \tag{20}$$

Thus m^* rises more rapidly with w than $\tilde{m}$, and the form (20) is not at first sight expected from relativity. Yet it does occur there when the acceleration is parallel (or antiparallel) to the velocity as the so-called "longitudinal" mass,[22] which satisfies precisely Eq. (20). Thus there is an analogy also in this case.

In addition to resonance effects,[2] experiments on relativistic plasmas can also be done in solids using the beneficial fact that $v \ll c$.[23,24] As no other relevant references have been found, one can say (perhaps surprisingly) that the systematic exposition of the basic principles of this pleasing analogy appears here for the first time.

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