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Reconciliation of the Conwell–Weisskopf and Brooks–Herring formulae for charged-impurity scattering in semiconductors: Third-body interference

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Abstract. The divergence at small scattering angles for unscreened charged-impurity scattering may be removed by including the probability that a closer scattering centre does not exist. This introduces an exponential function like the screening factor, which allows a straightforward bridging to be made between non-screening and screening situations. An expression for the mobility which encompasses the Conwell–Weisskopf and Brooks–Herring results is derived.

The problem of the scattering of an electron by a random distribution of charged centres is one of some importance in connection with the mobility of electrons in semiconductors, especially at low temperatures. Over a wide range of conditions, the Born approximation and an essentially two-body model is thought to be a reasonably valid approach. One of the difficulties is the well-known divergence of the cross section for the scattering off a Coulombic centre at small scattering angles, clearly caused by the preponderance of collisions with, in classical terms, a large impact parameter. Such a catastrophe was avoided by Conwell and Weisskopf (1950) by arbitrarily cutting off the Coulomb field at a radius equal to half the mean distance apart of the scattering centres. Arbitrariness was avoided by Mott (1936) and in semiconductors by Brooks and Herring (1951) by introducing another physical feature, namely screening, into the model and thereby causing the scattering potential to fall off with distance more rapidly than in the purely Coulombic case. (See also Dingle (1955), Mansfield (1956), Takimoto (1959), March and Murray (1962), Hall (1962), Moore (1967), Falicov and Cuevas (1967) and Csavinsky (1976), for developments connected with the Brooks–Herring formula.) On the whole, the Brooks–Herring (BH) formula was preferred over the Conwell–Weisskopf (CW) formula, but it was always clear that where screening electrons were plainly not available, as in many situations at low temperatures, the BH approach fails and the CW formula becomes the only viable replacement. It is the purpose of this paper to point out that this unsatisfactory situation is a direct consequence of a simple logical omission in the basic model, as recently discussed for the case of Rutherford scattering (Ridley 1976).

The BH model relies on screening to limit the range of the scattering potential surrounding any one centre, and thereby to make a two-body approach possible. Thus screening not only guarantees a finite cross section, it also allows the scattering problem to be reduced to scattering by a single centre, provided the distance apart of the scattering centres is large compared with the screening length. When the latter condition is not met, the BH formula fails.

The CW model, on the other hand, tackles directly the problem of scattering by many centres, and reduces the problem to one of scattering by a single centre by assuming that the scattering effects of all lying further away than half the average distance separating the centres add up to zero, and only the nearest centre is operative.

There are two things in common in these approaches. Each model defines a characteristic length which defines the range of the scattering potential—screening length in the case of BH, half the average separation of centres in the case of CW. Each makes the assumptions that within the characteristic length there is only one centre, only that centre scatters and all other centres produce no effect. The essence of our approach is to quantify the assumption that only one centre is active, by introducing the probability that no second centre interferes. If a consistent one-centre scattering approximation is to be adopted, it would seem logically necessary to do this. It will be shown that this brings in an exponential function like the screening factor and allows a reconciliation of the BH and CW approaches.

The matter is best discussed in terms of the classical impact parameter. If the scattering is to be a two-body process, then only the closest scattering centre must be deemed to be effective and the effect of all others put equal to zero (on the grounds that all the individual forces add vectorially to zero because of the random distribution, except for the closest). But then it is necessary to weigh the differential cross section for scattering through an angle θ by the probability $P(b)$, where b is the impact parameter associated with the angle θ, of there being no scattering centre with impact parameter less than b. If such a third body existed then in our two-body model our original centre is ineffective, a phenomenon we may call third-body interference. The probability is given by (see the Appendix)

$$P(b) = \exp(-\pi b^2 Na), \tag{1}$$

where a is the average distance between centres and N the density of scattering centres. Thus, in the simple unscreened case, the differential cross section becomes

$$\sigma(\theta) = \frac{R^2 \exp[-\pi N a_0 R^2 \cot^2(\theta/2)]}{4\sin^4(\theta/2)}, \tag{2}$$

where θ is the angle through which the particle is scattered, $R = Ze^2/4\pi\epsilon m v^2$, Ze is the charge on the centre, ϵ the permittivity, m the mass of electron being scattered and v its velocity. The rapidly decreasing probability of a two-body scattering event at increasing impact parameters removes the divergence totally.

In the unscreened case, both classical and quantum theory give the same result for the differential cross section. The probability factor $P(b)$, however, is obtained essentially in classical terms. We will continue to employ classical ideas to calculate $P(b)$ in the screened case. This requires us first to obtain a relation between the impact parameter and the scattering angle, which is no longer given by $b = R\cot(\theta/2)$. We do this by employing the basic relationship between differential cross section and impact parameter, namely

$$\sigma(\theta)\mathrm{d}\Omega = 2\pi b|\mathrm{d}b|, \tag{3}$$

where, for the case of screening (e.g. Smith 1964),

$$\sigma(\theta) = \frac{R^2}{4}[\sin^2(\theta/2) + \beta^{-1}]^{-2}, \tag{4}$$

$d\Omega$ is the elementary solid angle into which the particle is scattered,

$$\beta^{-1} = \frac{h^2}{4m^{*2}v^2\lambda_D^2} \tag{5}$$

and λ_D is the Debye screening length. From equations (3) and (4) we obtain

$$b^2 = \frac{R^2(1 - x^2)}{(x^2 + \beta^{-1})(1 + \beta^{-1})}, \tag{6}$$

where $x = \sin(\theta/2)$, and consequently we take as the probability of there being no third-body interference to be given by equation (1) with b^2 given by equation (6). Thus our differential cross section becomes

$$\sigma(\theta) = \frac{R^2}{4}(x^2 + \beta^{-1})^{-2} \exp\{-\pi R^2 Na(1 - x^2)/[(x^2 + \beta^{-1})(1 + \beta^{-1})]\}, \tag{7}$$

which does not diverge at small angles even if screening is weak ($\beta \to \infty$).

We now proceed to calculate the mobility associated with this cross section for the usual case of non-degenerative statistics and parabolic, spherical band structure, in exactly the way the BH formula is calculated. We obtain

$$\mu = \mu_0 L^{-1}, \tag{8}$$

where

$$\mu_0 = \frac{64\pi^{1/2}\varepsilon^2(2kT)^{3/2}}{NZ^2e^3m^{*1/2}} \tag{9}$$

and L, the analogue of the logarithmic term in the BH and CW expressions, is given by

$$L = \exp[\alpha\beta/(1 + \beta)]\left(E_1(\alpha\beta/(1 + \beta)) - E_1(\alpha\beta) - \frac{\exp[-\alpha\beta/(1 + \beta)]}{\alpha\beta} + \frac{\exp(-\alpha\beta)}{\alpha\beta}\right), \tag{10}$$

where

$$\alpha = Z^2e^4Na/576\pi\varepsilon^2(kT)^2, \tag{11}$$

$$\beta = 24m^*\varepsilon(kT)^2/e^2\hbar^2N_s, \tag{12}$$

$$\alpha\beta = Z^2e^2m^*Na/24\pi\varepsilon\hbar^2N_s \tag{13}$$

and $E_1(z)$ is the exponential integral. (β is the expression given by equation (5) with $\frac{1}{2}m^*v^2 = 3kT$.) N_s is the screening density of electrons, free and trapped. Three regions can be defined:

(i) $\alpha\beta \ll 1$ (screened)

$$L \to \ln(1 + \beta) - \frac{\beta}{1 + \beta} \tag{14}$$

and hence we retrieve the Brooks–Herring formula exactly.

(ii) $1 \ll \alpha\beta \ll 1 + \beta$ (unscreened, dilute)

$$L \to \ln(\alpha e^{\gamma})^{-1}, \tag{15}$$

where γ is Euler's constant. Choosing the average distance apart of scattering centres to be given by

$$a = (4/\pi)e^{-\gamma}N^{-1/3}, \tag{16}$$

we retrieve the Conwell–Weisskopf formula (apart from an insignificant additive factor of unity in the logarithm).

(iii) $\underline{1 + \beta \ll \alpha\beta}$ (unscreened, concentrated)

$$L \to \alpha^{-1}. \tag{17}$$

However, equation (8) is valid only if L is weakly dependent on average electron energy. This is the case for the BH and CW regimes, but not for this condition, which corresponds to the situation in which the total momentum-change cross section, σ_c, turns out to be independent of electron energy, namely

$$\sigma_c = \frac{2}{Na}. \tag{18}$$

Working out the mobility for this case leads to

$$\mu = \frac{\sqrt{2}ea}{3(\pi m^* kT)^{1/2}} \tag{19}$$

(which is bigger than that derived from equation (8) with equations (17) and (11) by a factor 3/2). This result agrees with the CW approach in the limit of large concentrations/small temperatures.

To sum up, the elimination of all but two-body scattering eliminates the catastrophe at zero scattering angle and allows us to derive a formula for the mobility limited by charged-impurity scattering in semiconductors which reconciles and encompasses the CW and

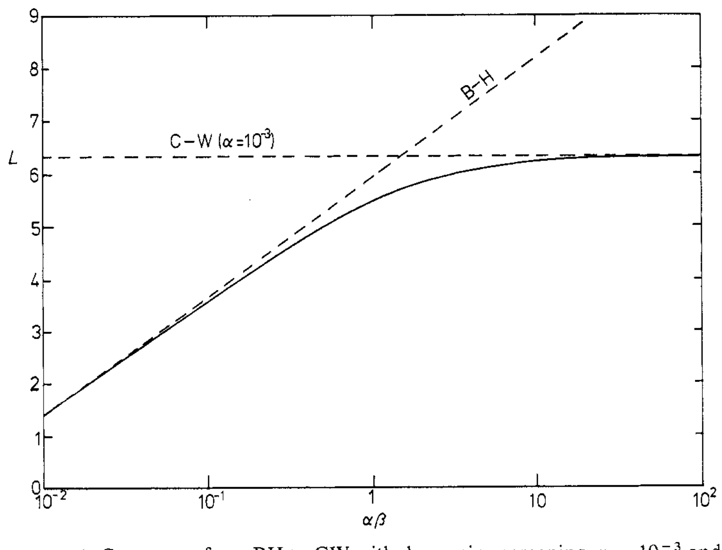

Figure 1. Cross-over from BH to CW with decreasing screening. $\alpha = 10^{-3}$ and L is the logarithmic factor in the expression for mobility (see text).

BH formulae. It is shown that the CW formula is valid when screening is weak ($\alpha\beta \gg 1$, regions (ii) and (iii)) and the BH formula is valid when screening is strong ($\alpha\beta \ll 1$). The practical utility of our result is to define a boundary between the unscreened and screened regions given by $\alpha\beta = 1$. It is the region near the boundary where our general expression is most useful. Figure 1 illustrates the cross-over from the screened limit (BH) to the unscreened limit (CW).

Appendix

To calculate $P(b)$ we note first of all that, if p denotes the probability of there being no centre with impact parameter between b and $b + \mathrm{d}b$, then

$$p = 1 - 2\pi Nab\mathrm{d}b,$$

since $2\pi Nab\mathrm{d}b$ is the probability that such a centre exists. Then, by the usual law of probabilities,

$$P(b + \mathrm{d}b) = P(b)p,$$

and therefore it follows that

$$P(b) = C\exp(-\pi Nab^2).$$

Since $P(O) = 1$, it follows that $C = 1$ and equation (1) is obtained.

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