Theory of Tunneling and its Dependence on a Longitudinal Magnetic Field*

PETROS N. ARGYRES
Lincoln Laboratory,† Massachusetts Institute of Technology, Lexington, Massachusetts
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A theory of interband tunneling due to a constant electric field is presented which is free of certain objections to previous theories. It is shown that the expression for the Zener current has new terms oscillatory in the electric field, which reflect the Stark quantization of the longitudinal motion of the electron. It is pointed out that for sufficiently small electric fields, the tunneling probability itself is an oscillatory function of the electric field. The effect of a longitudinal magnetic field on the tunneling is calculated for a class of substances. The tunneling in InSb in a magnetic field is considered in detail. Effects of spin-orbit interaction and nonparabolicity of energy bands are taken into account.

1. INTRODUCTION

THIS paper is concerned primarily with the calculation of the effect of a magnetic field on the interband tunneling in solids due to a uniform longitudinal electric field. Such an effect has been recently observed by Calawa *et al.*[1] and Chynoweth *et al.*[2] in InSb and by Rediker *et al.*[3] in PbTe. Elementary theories of this effect have been given by Calawa *et al.*,[1] Haering and Adams,[4] and Argyres and Lax,[5] where simplifying assumptions about band structure and matrix elements were made. This paper presents a more quantitative theory of magneto-tunneling for substances whose energy band structure in the presence of a magnetic field can be adequately described within the approximations discussed by Yafet.[6]

The calculation of the direct-tunneling probability is formulated along lines parallel to those of Kane's[7] recent work. Since, however, certain objections to this procedure have been raised by Kane himself[7] and by Price and Radcliffe,[8] an alternative presentation of the theory of direct tunneling is given first in the next section, in which these objections are discussed and removed by a more detailed consideration of time-dependent perturbation theory. This provides, in addition, a more accurate description of the Zener current, in which the Stark quantization[9] of the electronic levels within a band is reflected as small-current oscillations with the electric field. The tunneling matrix element is discussed and it is pointed out that under certain circumstances it is an oscillatory function of the electric field. Quantities such as transition probability rates per electron and transmission coefficients for an Esaki diode are then deduced in a *quasi-classical* approximation.

The theory of direct tunneling in a longitudinal magnetic field is presented in Sec. 3. It is pointed out that the most reliable way to calculate the effect of the magnetic field on the tunneling is to determine first the band structure of the substance in the magnetic field. Yafet's[6] results on the approximate energy levels and eigenfunctions of an electron in a periodic potential and a magnetic field are first summarized in a form convenient for our purposes. For completeness, these results are obtained briefly in the Appendix by a direct procedure which avoids the use of the Luttinger-Kohn[6,10] representation. The theory of tunneling is developed then briefly, as in Sec. 2, and the important matrix element that determines the tunneling is derived.

The last section deals with the application of the previous results to InSb. The band structure of this substance is taken to be that discussed by Kane[11] and used by Bowers and Yafet[12] in their study of its magnetic susceptibility. The effects of spin-orbit interaction and spin, as well as those of the nonparabolicity of the energy bands are taken into consideration. Only the dominant tunneling among the light-hole valence and conduction bands is evaluated explicitly. It turns out that for InSb in this approximation the main effect of the magnetic field is given by the quantization of the transverse energy and the subsequent increase of the effective energy gap, which results in a decrease of the tunneling probability.

Finally, it must be remarked that existing theories of interband tunneling are far from rigorous. A number of implicit statistical assumptions are made which can be eliminated only if collisions are taken into consideration from the beginning.

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2. THEORY OF INTERBAND TUNNELING

In this section, a theory of the Zener current in the absence of a magnetic field is presented, in order primarily to remove the objections of Kane[7] and Price and Radcliffe[8] mentioned earlier.

The eigenfunctions of an electron of the crystal in a uniform force field F in the z direction and in the energy band α are[7,9]

$$\phi_{\nu\mathbf{k}_\perp}{}^{\alpha}(\mathbf{r})=\sum_{k_z} A_\nu{}^{\alpha}(\mathbf{k})\psi_{\alpha\mathbf{k}}(\mathbf{r}), \tag{2.1}$$

with energy $W_\nu{}^{\alpha}$. Here $\psi_{\alpha\mathbf{k}}$ are the Bloch states and $A_\nu{}^{\alpha}(\mathbf{k})$ and $W_\nu{}^{\alpha}$ are eigenfunctions and eigenvalues given by

$$[E_\alpha(\mathbf{k})-iF\partial/\partial k_z]A_\nu{}^{\alpha}(\mathbf{k})=W_\nu{}^{\alpha}A_\nu{}^{\alpha}(\mathbf{k}), \tag{2.2}$$

where $E_\alpha(\mathbf{k})$ is the energy of the Bloch state $\psi_{\alpha\mathbf{k}}$ increased by $(-F)Z_{\alpha\alpha}(\mathbf{k})$, $Z_{\alpha\alpha'}(\mathbf{k})$ being the diagonal-in-$\mathbf{k}$ matrix element of z in the Bloch states $\psi_{\alpha\mathbf{k}}$, $\psi_{\alpha'\mathbf{k}}$. If the direction of the electric field is along *any* one of the (infinite) vectors of the reciprocal lattice, the first Brillouin zone can be so chosen that the end points of k_z differ by a reciprocal lattice vector and thus denote the same state. Equation (2.2) is subjected then to periodic boundary conditions and thus it is found that

$$A_\nu{}^{\alpha}(\mathbf{k})=\kappa^{-\frac{1}{2}}\exp\left\{\frac{i}{F}\int_0^{k_z}[W_\nu{}^{\alpha}-E_\alpha(\mathbf{k}_\perp k_z')]dk_z'\right\}, \tag{2.3}$$

$$W_\nu{}^{\alpha}(\mathbf{k}_\perp)=\nu\frac{2\pi F}{\kappa}+\frac{1}{\kappa}\int_{-\kappa/2}^{\kappa/2}E_\alpha(\mathbf{k}_\perp k_z')dk_z', \tag{2.4}$$

where κ is the width of the Brillouin zone in the z direction. Here ν is an integer which denotes the Stark quantization of the motion of the electron within one band in the presence of a constant electric field. The states as described by (2.1) and (2.3) are orthonormal if the Bloch states $\psi_{\alpha\mathbf{k}}$ are taken to be orthonormal.

The complete motion of the electron is, of course, described by the Schrödinger equation

$$i\hbar d\psi/dt=(\mathcal{H}_0-Fz)\psi, \tag{2.5}$$

where $\mathcal{H}_0$ is the unperturbed crystal Hamiltonian. If it is assumed that the wave function $\psi(t)$ can be adequately described as a superposition of the $\phi_{\nu\mathbf{k}_\perp}{}^{\alpha}$'s, i.e., if

$$\psi(t)=\sum_{\alpha\nu\mathbf{k}_\perp} b_{\nu\mathbf{k}_\perp}{}^{\alpha}(t)\phi_{\nu\mathbf{k}_\perp}{}^{\alpha}, \tag{2.6}$$

it is found quite generally that the transverse-wave vector $\mathbf{k}_\perp$ is conserved in the interband transitions. In particular, if an electron was in the state $\phi_{\nu'\mathbf{k}_\perp}{}^{\alpha'}$ at $t=0$, the probability of finding it in the state $\phi_{\nu\mathbf{k}_\perp}{}^{\alpha}$ at time t is, to the lowest order in the interband interaction,

$$|b_{\nu\mathbf{k}_\perp}{}^{\alpha}(t)|^2=(F/\hbar\kappa)^2|M_{\alpha\alpha'}(\mathbf{k}_\perp\nu\nu')|^2 \times\Omega[W_\nu{}^{\alpha}(\mathbf{k}_\perp)-W_{\nu'}{}^{\alpha'}(\mathbf{k}_\perp),t], \tag{2.7}$$

where

$$M_{\alpha\alpha'}(\mathbf{k}_\perp\nu\nu')=\kappa\int_{-\kappa/2}^{\kappa/2}A_\nu{}^{\alpha*}(\mathbf{k})Z_{\alpha\alpha'}(\mathbf{k})A_{\nu'}{}^{\alpha'}(\mathbf{k})dk_z \tag{2.8}$$

and $\Omega[s,t]=4(s/\hbar)^{-2}\sin^2(st/2\hbar)$. It is clear that, since the transverse-wave vector $\mathbf{k}_\perp$ is conserved in the transition and the quantum number ν is discrete even for an infinite crystal, there is no transition probability rate for transitions from a definite state.

The number, however, of electrons (per unit volume) that tunnel to the empty band α from the full band α' per unit time is given by

$$w_{\alpha\alpha'}=\frac{1}{t}\frac{2}{L_z}\sum_\nu\sum_{\nu'}\int\frac{d\mathbf{k}_\perp}{(2\pi)^2}|b_{\nu\mathbf{k}_\perp}{}^{\alpha}(t)|^2, \tag{2.9}$$

where L_z is the length of the specimen in the z direction. (The factor 2 takes account of the spin.) Within the integral (2.9) $\Omega[s,t]$ can be taken in the usual manner to be, for long times, a delta function and thus

$$w_{\alpha\alpha'}=\frac{2}{L_z}\frac{2\pi}{\hbar}\frac{F^2}{\kappa^2}\sum_\nu\sum_{\nu'}\int\frac{d\mathbf{k}_\perp}{(2\pi)^2}|M_{\alpha\alpha'}(\mathbf{k}_\perp)|^2 \times\delta[W_\nu{}^{\alpha}(\mathbf{k}_\perp)-W_{\nu'}{}^{\alpha'}(\mathbf{k}_\perp)], \tag{2.10}$$

where now, because of the delta function and (2.3),

$$M_{\alpha\alpha'}(\mathbf{k}_\perp)=\int_{-\kappa/2}^{\kappa/2}Z_{\alpha\alpha'}(\mathbf{k}) \times\exp\left\{\frac{i}{F}\int_0^{k_z}E_{\alpha\alpha'}(\mathbf{k}_\perp k_z')dk_z'\right\}dk_z, \tag{2.11}$$

which is independent of the quantum numbers ν and ν'. Here $E_{\alpha\alpha'}$ stands for $E_\alpha-E_{\alpha'}$.

The objections[7,8] to Kane's[7] treatment of the same problem refer to the use of the concept of a transition probability rate per state, which, as we saw above, is not applicable due to the structure of the energy spectrum and the selection rule for tunneling. These objections do not apply to the present treatment, since for the quantity $w_{\alpha\alpha'}$ the initial distribution of electrons provides the continuum of levels necessary for the standard use of the concept of a transition rate. The situation here is similar to that of interband transitions due to absorption of photons.

Statistical assumptions about repeated random phases and initial distribution of electrons are, however, still tacitly made. Only a simultaneous consideration of collisions can put the theory on a firmer theoretical basis.

A more explicit form can be given for $w_{\alpha\alpha'}$. From (2.4) it is clear that the summand in (2.10) depends on ν and ν' only through their difference $\nu-\nu'$. The summations may be chosen to range over the integers $0, 1, \cdots, N$, where N is a large integer of the order of $(\kappa L_z)/2\pi$. Now,

it is easily proved that for a function $f(x)$ possessing a Fourier transform

$$\sum_{\nu=0}^{N}\sum_{\nu'=0}^{N} f(\nu-\nu')=\int_{-\infty}^{+\infty} d\lambda\, g(\lambda)\frac{\sin^2[(N+1)\lambda/2]}{\sin^2(\lambda/2)}, \quad (2.12)$$

where $g(\lambda)$ is the Fourier transform of $f(x)$, i.e.,

$$g(\lambda)=\frac{1}{2\pi}\int_{-\infty}^{+\infty} f(x)e^{i\lambda x}dx. \quad (2.13)$$

In our case $f(\nu-\nu')$, given by the integral over $\mathbf{k}_\perp$ in (2.10), will always have a Fourier transform, since for large $|\nu-\nu'|$ it is zero, on account of the δ function and the boundedness of $E_\alpha(\mathbf{k})$. Since for large N

$$\frac{\sin^2[(N+1)\lambda/2]}{\sin^2(\lambda/2)}=2\pi N\sum_{m=-\infty}^{+\infty}\delta(\lambda-2\pi m), \quad (2.14)$$

it is evident that for a large specimen

$$\frac{1}{L_z}\sum_{\nu}\sum_{\nu'} f(\nu-\nu')=\frac{\kappa}{2\pi}\sum_{m=-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x)e^{i2\pi mx}dx. \quad (2.15)$$

In Eq. (2.10) for $w_{\alpha\alpha'}$ the difference $\nu-\nu'$ occurs only in the argument of the delta function and thus the integrations over x in (2.15) can be carried out immediately, thus yielding

$$w_{\alpha\alpha'}=\frac{2|F|}{(2\pi)^3\hbar}\Big[\int|M_{\alpha\alpha'}(\mathbf{k}_\perp)|^2 d\mathbf{k}_\perp + 2\sum_{m=1}^{\infty}\int|M_{\alpha\alpha'}(\mathbf{k}_\perp)|^2\cos\Big(m\frac{\Delta_{\alpha\alpha'}(\mathbf{k}_\perp)}{F/\kappa}\Big)d\mathbf{k}_\perp\Big], \quad (2.16)$$

where

$$\Delta_{\alpha\alpha'}(\mathbf{k}_\perp)=(1/\kappa)\int_{-\kappa/2}^{\kappa/2} E_{\alpha\alpha'}(\mathbf{k}_\perp k_z')dk_z'. \quad (2.17)$$

The first term in (2.16) is just the result obtained by Kane[7] by use of an average smoothed-out density of states. The additional terms describe the effect of the Stark quantization of the energy levels within one band. They are in general oscillatory functions of the electric field. The amplitudes of these oscillations are in general small compared to the main term, their relative magnitude being in a typical case of the order of [(energy gap)/(sum of energy-band widths)]$^{\frac{1}{2}}$.[13] The existence of collisions will drastically diminish these oscillatory terms, since for all but the lowest temperatures the collision frequency is much higher than the Bohr frequency associated with the spacing of the Stark levels.

The matrix element $M_{\alpha\alpha'}$, Eq. (2.11), has been evaluated by several authors for small values of F by a technique similar to the method of stationary phase, yielding an exponentially decreasing function of $1/F$. It is worthwhile to point out that this evaluation does *not* yield the asymptotic value of the integral for small F. The asymptotic value for arbitrary $\mathbf{k}_\perp$ can be found by an integration by parts[14]; for nonoverlapping bands, i.e., $E_{\alpha\alpha'}(\mathbf{k})\neq 0$, it is

$$M_{\alpha\alpha'}(\mathbf{k}_\perp)\sim 2F\frac{Z_{\alpha\alpha'}(\mathbf{k}_\perp,\kappa/2)}{E_{\alpha\alpha'}(\mathbf{k}_\perp,\kappa/2)}\sin\Big(\frac{\Delta_{\alpha\alpha'}(\mathbf{k}_\perp)}{2F/\kappa}\Big)+O(F^2). \quad (2.18)$$

This is seen to be a product of an oscillatory and a linear function of the electric field, so that for sufficiently small F, it is dominant over the contribution to the integral of the stationary phase point. However, for electric fields strong enough to produce substantial Zener currents, it is possible that the contribution to the integral for $M_{\alpha\alpha'}$ of the stationary-phase point is larger than that of the end points. For InSb we have estimated, on the basis of the two-band model of Kane, that for electric fields of the order of 10^4 v/cm the contribution of the stationary-phase point is by far the dominant. The two contributions should, however, be compared separately for each case due to the fairly large range of the values of the parameters involved. It should be observed that the oscillatory dependence of the tunneling matrix element $M_{\alpha\alpha'}(\mathbf{k}_\perp)$, as given by (2.18), on the electric field is *not* due to the Stark quantization of the electronic motion. The effects of this quantization on the Zener current are fully described by the additional terms in (2.16) and were discussed above. It must also be noted that for the $\mathbf{k}_\perp$ conserving energy on the tunneling process the asymptotic evaluation (2.18) of $M_{\alpha\alpha'}(\mathbf{k}_\perp)$ makes no contribution to the Zener current, as it can be seen from Eq. (2.10), due to the identity of the $-\kappa/2$ and $\kappa/2$ points. Eq. (2.18) is of interest, however, in the case of an Esaki diode, if the quasi-classical treatment of it given in the next paragraph is valid.

For the case of an Esaki diode, where the electric field (presumed constant) is localized in a small region, one is interested in the transmission coefficient. This

[13] This can be seen as follows: For the simple case of two parabolic bands with an energy gap ϵ_g (at $\mathbf{k}=0$) and reduced effective mass m_r, it can be seen from (2.11) that for electric-field strengths of interest (cf. following paragraph) the essential dependence of $M_{\alpha\alpha'}$ on $\mathbf{k}_\perp$ is given by

$$M(\mathbf{k}_\perp)\cong M(0)\exp(-\beta k_\perp^2),$$

where $\beta=(\hbar/|F|)(\epsilon_g/2m_r)^{\frac{1}{2}}$. [See also reference 7 and Eqs. (4.11) and (4.12).] Similarly, Eq. (2.17) gives for the same case

$$\Delta(\mathbf{k}_\perp)=\Delta(0)+(\hbar^2/2m_r)k_\perp^2.$$

Thus, the ratio of the mth oscillatory to the steady term of Eq. (2.16) is found to be approximately

$$\frac{2(A/m)}{1+(A/m)^2}\Big[\Big(\frac{A}{m}\Big)\cos\Big(\frac{m\Delta(0)}{F/\kappa}\Big)-\sin\Big(\frac{m\Delta(0)}{F/\kappa}\Big)\Big],$$

where

$$|A|=\beta\frac{|F|/\kappa}{\hbar^2/2m_r}=\Big(\frac{\epsilon_g}{\hbar^2\kappa^2/2m_r}\Big)^{\frac{1}{2}}\cong\frac{1}{2}\Big(\frac{\text{energy gap}}{\text{sum of energy band widths}}\Big)^{\frac{1}{2}}.$$

Therefore, for $|A|\ll 1$ the relative order of magnitude of the amplitude of the oscillatory terms is $\sim 2A$.

[14] See, e. g., A. Erdélyi, *Asymptotic Expansions* (Dover Publications, New York, 1956), p. 47.

can be deduced from (2.16) by the following *quasi-classical* reasoning. Since the density of electrons in a band with transverse wave numbers between $\mathbf{k}_\perp$, $\mathbf{k}_\perp+d\mathbf{k}_\perp$ is $2\kappa d\mathbf{k}_\perp/(2\pi)^3$, Eq. (2.16) may be interpreted to give for the probability rate for tunneling of an electron with transverse-wave number $\mathbf{k}_\perp$ the quantity

$$P_{\alpha\alpha'}(\mathbf{k}_\perp)=(|F|/\hbar\kappa)|M_{\alpha\alpha'}(\mathbf{k}_\perp)|^2. \quad (2.19)$$

Now, since the electron oscillates within the band along the z direction with frequency $|F|/\hbar\kappa$, the transmission coefficient for such an electron is

$$D_{\alpha\alpha'}(\mathbf{k}_\perp)=(\hbar\kappa/|F|)P_{\alpha\alpha'}(\mathbf{k}_\perp)=|M_{\alpha\alpha'}(\mathbf{k}_\perp)|^2. \quad (2.20)$$

The oscillatory terms in (2.16), which are the result of the quantized motion of the electron in the z direction, should be ignored in this quasi-classical argument. This is so because in a diode where the band gap is much smaller than the band widths the motion of the electron in its band is unquantized, since it is spatially unlimited in the direction away from the junction. A more explicit consideration of the transmission coefficient for an Esaki diode yields, in a quasi-classical approximation, the same result. No strict quantum-mechanical treatment has been given yet, however.

It should, perhaps, be stated explicitly that these considerations make it clear that in a tunnel diode any oscillations of the tunnel current with the electric field cannot be attributed to the Stark quantization of the electronic motion, as Chynoweth *et al.*[15] have erroneously done. In cases, however, where the evaluation (2.18) of the tunneling matrix element is applicable, oscillations of the tunnel current with the electric field are possible if the previous quasi-classical argument is valid. It has not, however, been investigated whether this is the case with the experimental situation of reference 15.

3. THEORY OF INTERBAND TUNNELING IN A LONGITUDINAL MAGNETIC FIELD

In this section a theory of the effect of a magnetic field on the direct tunneling due to a constant longitudinal electric field is presented on the basis of an approximation sufficiently good for application to InSb.

Formally the phenomenon of tunneling of an electron in a solid due to an electric field is connected with the fact that the interaction with the electric field has nonvanishing interband matrix elements. Although as Kane[7] pointed out, these can be eliminated to any order of the electric field by a redefinition of the energy bands, there is always an interband matrix element of higher order which brings about tunneling between the modified energy bands. The modification of the bands is of negligible importance as far as tunneling is concerned.

The presence of a magnetic field complicates matters, because its interaction with the electron also has interband matrix elements. The simplest way, therefore, to calculate reliably the effect of a magnetic field on the tunneling and separate it from spurious effects is to determine first the energy-band structure of the electron in the presence of the magnetic field and then investigate the tunneling among these new bands.

Determination of the energy spectrum and eigenfunctions of an electron in a periodic potential and a magnetic field is quite complicated. The effective-mass approximation is not sufficiently good for our purposes. A better approximation, in which the interband matrix elements of the magnetic interaction among a number of energetically close bands are eliminated exactly, has been presented by Yafet.[6] This gives the energy levels and eigenfunctions in the approximation of (a) negligible lattice broadening and (b) spherical energy bands or s and p bands in a cubic crystal (e.g., InSb).

The results of this approximation, which are obtained by a more direct method in the Appendix, may be summarized as follows. For a magnetic field H in the z direction, described by the vector potential $\mathbf{A}=(0,Hx,0)$, the orthonormalized (in volume V) eigenfunctions of the complete Hamiltonian, including the spin-orbit and Zeeman energies, are

$$\psi_{nk_yk_z}{}^{\alpha}(\mathbf{r})=\frac{\sqrt{V}}{2\pi}e^{ik_yy}e^{ik_zz}\sum_{\mu}C_\mu{}^{\alpha}(nk_z)\times\Phi_{n-m(\mu)}\left(x+\frac{\hbar k_y}{m\omega}\right)u_\mu(\mathbf{r}), \quad (3.1)$$

with eigenvalues $E_\alpha(nk_z)$. Here $n[\geq m(\mu)]$ is an integral quantum number designating the Landau levels and α denotes the bands in the presence of the magnetic field. Φ_n are the simple harmonic oscillatory eigenfunctions, ω stands for the free-electron cyclotron frequency, and $u_\mu(\mathbf{r})$ are the periodic parts of the Bloch wave functions for $\mathbf{k}=0$ for the unperturbed (no magnetic field) problem, i.e., they are 2 spinors (orthonormalized in the unit cell) such that

$$\mathcal{H}_0u_\mu(\mathbf{r})=\mathcal{E}_\mu u_\mu(\mathbf{r}), \quad u_\mu(\mathbf{r}+\mathbf{R})=u_\mu(\mathbf{r}). \quad (3.2)$$

The summation on μ extends over a number of energetically close unperturbed bands deemed sufficient to provide a desired approximation. $m(\mu)$ are integers characterizing the unperturbed bands μ, so that under approximation (b) the matrix elements of the unperturbed velocity operators v^z, $v^\pm=\frac{1}{2}(v^x\pm iv^y)$ and the Zeeman energy operator $\epsilon=(1/2)g_s\beta H\sigma_z$ in the representation of the u_μ's obey the following selection rules

$$v_{\mu\mu'}{}^z,\ \epsilon_{\mu\mu'}\propto\delta_{m(\mu),m(\mu')};\ v_{\mu\mu'}{}^\pm\propto\delta_{m(\mu),m(\mu')\pm1}. \quad (3.3)$$

Finally, the coefficients $C_\mu{}^\alpha(nk_z)$ and the energy eigenvalues $E_\alpha(nk_z)$ are given as the orthonormalized eigenvectors and eigenvalues of the Hermitian matrix

[15] A. G. Chynoweth, G. H. Wannier, R. A. Logan, and D. E. Thomas, Phys. Rev. Letters 5, 57 (1960).

$L_{\mu\mu'}(nk_z)$, i.e.,

$$\sum_{\mu'} (L_{\mu\mu'}-E\delta_{\mu\mu'})C_{\mu'}=0, \tag{3.4}$$

where

$$L_{\mu\mu'}=\left\{\mathcal{E}_\mu+\frac{\hbar^2k_z^2}{2m}+[n-m(\mu)+\tfrac{1}{2}]\hbar\omega\right\}\delta_{\mu\mu'} +\hbar k_z v_{\mu\mu'}{}^z+\epsilon_{\mu\mu'}+i(2m\hbar\omega)^{\frac{1}{2}} \times\{v_{\mu\mu'}{}^-[n-m(\mu)]^{\frac{1}{2}}-v_{\mu\mu'}{}^+[n-m(\mu)+1]^{\frac{1}{2}}\}. \tag{3.5}$$

The interband tunneling due to a uniform force field F parallel to the magnetic field is computed as in the previous section. First the intraband effects of the electrostatic interaction $-Fz$ are treated exactly and then the interband matrix elements are handled by time-dependent perturbation theory. The matrix elements of z among the $\psi_{nk_yk_z}{}^\alpha$ of (3.1) can now be found by an integration by parts to be (apart from terms of the same order as those causing lattice broadening)

$$(\psi_{nk_yk_z}{}^\alpha,z\psi_{n'k_y'k_z'}{}^{\alpha'})=\delta_{\alpha\alpha'}\delta_{nn'}\delta_{k_yk_y'}\frac{1}{i}\frac{\partial}{\partial k_z'}\delta(k_z'-k_z) +Z_{\alpha\alpha'}(nk_z)\delta_{nn'}\delta_{k_yk_y'}\delta_{k_zk_z'}, \tag{3.6}$$

where

$$Z_{\alpha\alpha'}(nk_z)=i\sum_\mu C_\mu{}^{\alpha*}(nk_z)\frac{\partial}{\partial k_z}C_\mu{}^{\alpha'}(nk_z). \tag{3.7}$$

From the form of the intraband elements in (3.6) it is clear that the eigenfunctions of the electron in the presence of the electric field and in the zeroth order of interband effects are, in close analogy to (2.1),

$$\phi_{\nu nk_y}{}^\alpha(\mathbf{r})=\sum_{k_z} A_\nu{}^\alpha(nk_yk_z)\psi_{nk_yk_z}{}^\alpha(\mathbf{r}) \tag{3.8}$$

with energies $W_\nu{}^\alpha$, where

$$[E_\alpha(nk_z)-iF\partial/\partial k_z]A_\nu{}^\alpha=W_\nu{}^\alpha A_\nu{}^\alpha. \tag{3.9}$$

In (3.9) the $(-F)Z_{\alpha\alpha}(nk_z)$ intraband matrix element has been absorbed in $E_\alpha(nk_z)$. As in the previous section, if the electric field is along any one of the reciprocal lattice vectors, Eq. (3.9) is subjected to periodic boundary conditions and then

$$A_\nu{}^\alpha(nk_yk_z)=\kappa^{-\frac{1}{2}}\exp\left\{\frac{i}{F}\int_0^{k_z}[W_\nu{}^\alpha(n)-E_\alpha(nk_z')]dk_z'\right\}, \tag{3.10}$$

$$W_\nu{}^\alpha(n)=\nu\frac{2\pi F}{\kappa}+\frac{1}{\kappa}\int_{-\kappa/2}^{\kappa/2}E_\alpha(nk_z')dk_z', \tag{3.11}$$

with ν an integer, describing as before the Stark quantization of the longitudinal motion due to the electric field.

It is easily seen that in the interband transitions the quantum numbers n and k_y of the transverse motion are conserved. The number of electrons that tunnel from a full band α' to an empty one α per unit volume and unit time is found by the procedure of the previous section to be

$$w_{\alpha\alpha'}(H)=\frac{|F|}{(2\pi)^2\hbar}\frac{eH}{\hbar c}\sum_n|M_{\alpha\alpha'}(n)|^2, \tag{3.12}$$

where

$$M_{\alpha\alpha'}(n)=\int_{-\kappa/2}^{\kappa/2}Z_{\alpha\alpha'}(nk_z) \times\exp\left\{\frac{i}{F}\int_0^{k_z}E_{\alpha\alpha'}(nk_z')dk_z'\right\}dk_z. \tag{3.13}$$

In (3.12) the additional small terms that are oscillatory functions of the electric field and result from the Stark quantization of the longitudinal motion have been ignored.

In a *quasi-classical* fashion the probability rate for tunneling for an electron in the n Landau level may be taken to be given by

$$P_{\alpha\alpha'}(n)=(|F|/\hbar\kappa)|M_{\alpha\alpha'}(n)|^2, \tag{3.14}$$

since the density of electrons in a band with a definite Landau quantum number is $\kappa(eH/\hbar c)/(2\pi)^2$. Similarly, since the frequency of oscillation within one band is unaffected by the longitudinal magnetic field, the transmission coefficient for an electron in the n Landau level can be taken in a *quasi-classical* approximation to be

$$D_{\alpha\alpha'}(n)=|M_{\alpha\alpha'}(n)|^2. \tag{3.15}$$

The remarks made in the last section about the evaluation of the tunneling matrix element as a function of the electric field are applicable also to the matrix element $M_{\alpha\alpha'}(n)$ given by (3.13).

The matrix element $M_{\alpha\alpha'}(n)$ for the interband tunneling is given in terms of $Z_{\alpha\alpha'}(nk_z)$, the interband matrix element of z, Eq. (3.7). The normalized $C_\mu{}^\alpha(nk_z)$ are, however, fairly complicated functions of k_z and expression (3.7) for $Z_{\alpha\alpha'}$ is cumbersome. A different expression for it can, however, be found in terms of the derivative of the matrix $L_{\mu\mu'}(nk_z)$, which is much simpler due to the simpler dependence of $L_{\mu\mu'}$ on k_z. Since $L_{\mu\mu'}$ is a Hermitian matrix with $C_\mu{}^\alpha$ and E_α its eigenvectors and eigenvalues, it is easily proved by standard techniques that for $\alpha'\neq\alpha$

$$Z_{\alpha\alpha'}(nk_z)=i\frac{\sum\sum_{\mu\mu'}C_\mu{}^{\alpha*}(nk_z)[\partial L_{\mu\mu'}(nk_z)/\partial k_z]C_{\mu'}{}^{\alpha'}(nk_z)}{E_{\alpha'}(nk_z)-E_\alpha(nk_z)}. \tag{3.16}$$

This expression will be used in the following application.

4. APPLICATION TO InSb

The following application is based on the band structure of InSb as calculated by Kane[11] and applied to a calculation of the magnetic susceptibility of its conduction electrons by Bowers and Yafet.[12] Only the

predominant tunneling among the conduction and light-hole valence bands will be evaluated explicitly. The magnetic field is taken for convenience to be along the [100] direction.

The energetically close bands are taken to be those arising from the s and p orbitals except for the spin-orbit split-off bands, i.e., in the notation of Kane,[11] we take $\Delta=\infty$. The remaining bands are characterized by the spinors $u_\mu(\mathbf{r})$ ($\mu=1, 2, \cdots 6$), taken to be identical to the first six used in Eq. (1) of reference 12. If the integers $m(\mu)=0, 1, -1, 0, 1, 2$ are assigned, respectively, to the bands $\mu=1, 2, 3, 4, 5, 6$, the selection rules (3.3) are satisfied and the matrix $L_{\mu\mu'}(nk_z)$ determining the coefficients C_μ^α and energy eigenvalues E_α is found to be

$$\begin{aligned}
&L_{11}=\epsilon_g+\epsilon_z+(n+\tfrac{1}{2})\hbar\omega,\\
&L_{13}=L_{31}{}^*=-iP[s(n+1)]^{\frac{1}{2}},\\
&L_{14}=L_{41}{}^*=L_{25}=L_{52}{}^*=(2/3)^{\frac{1}{2}}Pk_z,\\
&L_{15}=L_{51}{}^*=L_{24}=L_{42}{}^*=-i(1/3)^{\frac{1}{2}}P(sn)^{\frac{1}{2}},\\
&L_{22}=\epsilon_g+\epsilon_z+(n-\tfrac{1}{2})\hbar\omega,\\
&L_{26}=L_{62}{}^*=iP[s(n-1)]^{\frac{1}{2}},\\
&L_{33}=\epsilon_z+(n+\tfrac{3}{2})\hbar\omega,\\
&L_{44}=\epsilon_z+(n+\tfrac{1}{2})\hbar\omega,\\
&L_{55}=\epsilon_z+(n-\tfrac{1}{2})\hbar\omega,\\
&L_{66}=\epsilon_z+(n-\tfrac{3}{2})\hbar\omega,
\end{aligned}\tag{4.1}$$

and all the others are equal to zero. Here, $\epsilon_z=\hbar^2k_z{}^2/2m$, $s=eH/\hbar c$, ϵ_g is the energy gap between the valence and conduction bands at $\mathbf{k}=0$ and P, in the notation of Kane,[11] is the interband velocity matrix element (multiplied by $\hbar$). In these expressions spin-orbit interaction has been taken into account up to first order and the Zeeman energy has been ignored because of its smallness. From (3.4) and (4.1) the energy eigenvalues for the conduction and light-hole valence bands are then found to be

$$E_{c\pm}(nk_z)=\frac{\epsilon_g}{2}+\frac{\epsilon_g}{2}\left\{1+\frac{8P^2}{3\epsilon_g{}^2}[k_z{}^2+2s(n\mp\tfrac{3}{4})]\right\}^{\frac{1}{2}},\tag{4.2}$$

$$E_{v\pm}(nk_z)=\frac{\epsilon_g}{2}-\frac{\epsilon_g}{2}\left\{1+\frac{8P^2}{3\epsilon_g{}^2}[k_z{}^2+2s(n\mp\tfrac{3}{4})]\right\}^{\frac{1}{2}}.\tag{4.3}$$

Energies are measured from the top of the valence band in the absence of the magnetic field. The ($\pm$) refer to the spin degree of freedom, but do not of course imply pure spin states. It is clear from these equations that the matrix element P can be written in terms of the effective masses at the band edges, namely,

$$P^2=3\hbar^2\epsilon_g/4m_c\ (|m_v|\cong m_c).$$

In (4.2) and (4.3) the additional term $\epsilon_z=\hbar^2k_z{}^2/2m$ has been ignored because it is much smaller than the effective mass term ($m_c\approx 0.013m$). Similarly, the normalized coefficients $C_\mu(nk_z)$ are given by

$$\begin{aligned}
&C_2{}^{\alpha+}=\{1+\tfrac{2}{3}(P/E_{\alpha+})^2[k_z{}^2+2s(n-\tfrac{3}{4})]\}^{-\frac{1}{2}},\\
&C_4{}^{\alpha+}=i(1/3)^{\frac{1}{2}}(P/E_{\alpha+})(sn)^{\frac{1}{2}}C_2{}^{\alpha+},\\
&C_5{}^{\alpha+}=(2/3)^{\frac{1}{2}}(P/E_{\alpha+})k_zC_2{}^{\alpha+},\\
&C_6{}^{\alpha+}=-i(P/E_{\alpha+})[s(n-1)]^{\frac{1}{2}}C_2{}^{\alpha+},\\
&C_1{}^{\alpha+}=C_3{}^{\alpha+}=0,
\end{aligned}\tag{4.4}$$

where α stands for either c or v. It should be observed that since $m(2)=1$, the Landau quantum number in the (+) bands ranges over the values $n=1, 2, 3, \cdots$. For the (−) bands the normalized coefficients are

$$\begin{aligned}
&C_1{}^{\alpha-}=\{1+\tfrac{2}{3}(P/E_{\alpha-})^2[k_z{}^2+2s(n+\tfrac{3}{4})]\}^{-\frac{1}{2}},\\
&C_3{}^{\alpha-}=i(P/E_{\alpha-})[s(n+1)]^{\frac{1}{2}}C_1{}^{\alpha-},\\
&C_4{}^{\alpha-}=(2/3)^{\frac{1}{2}}(P/E_{\alpha-})k_zC_1{}^{\alpha-},\\
&C_5{}^{\alpha-}=i(1/3)^{\frac{1}{2}}(P/E_{\alpha-})(sn)^{\frac{1}{2}}C_1{}^{\alpha-},\\
&C_2{}^{\alpha-}=C_6{}^{\alpha-}=0,
\end{aligned}\tag{4.5}$$

where now, since $m(1)=0$, $n=0, 1, 2, \cdots$.

For the calculation of the tunneling probability between the (+) bands the quantity Z_{c+v+} is obtained from Eqs. (3.16), (4.1), (4.2), (4.3), and (4.4). It is found to be

$$Z_{c+v+}(nk_z)=\frac{ik_z}{B}\left(1+\frac{8}{3}\frac{P^2}{\epsilon_g{}^2}B\right)^{-\frac{1}{2}}\times\left(1+\frac{2}{3}\frac{P^2}{E_{v+}{}^2}B\right)^{-\frac{1}{2}}\left(1+\frac{2}{3}\frac{P^2}{E_{c+}{}^2}B\right)^{-\frac{1}{2}},\tag{4.6}$$

where $B=k_z{}^2+2s(n-3/4)$. Advantage has been taken of the fact that $\partial L_{\mu\mu}/\partial k_z$ is independent of μ and of the orthogonality relation $\sum_\mu C_\mu{}^{\alpha*}C_\mu{}^{\alpha'}=\delta_{\alpha\alpha'}$. The matrix element $M_{c+v+}(n)$ is now obtained from Eqs. (3.13) and (4.6). For the electric-field strengths of interest the major contribution to the integral (3.13) comes, as it was discussed in the second section, from the neighborhood of the stationary-phase point in the complex k_z plane. From (4.2) and (4.3) the point of stationary phase is given by

$$q_0=\pm i[(3/8)(\epsilon_g/P)^2+2s(n-3/4)]^{\frac{1}{2}}.\tag{4.7}$$

In the neighborhood of q_0, i.e., for $k_z=q_0+q$ with q small, Eq. (4.6) yields after some algebra the simple form

$$Z_{c+v+}(n, q_0+q)=-1/4q,\tag{4.8}$$

and the oscillatory factor in the integrand of (3.13) is

$$\exp\left\{\frac{i}{F}\left[(\pm i)\frac{\pi P}{\sqrt{6}}|q_0|^2+\frac{8Pq_0{}^{\frac{1}{2}}}{3\sqrt{3}}q^{\frac{3}{2}}\right]\right\}.\tag{4.9}$$

Upon changing the contour of the integral (3.13) in the appropriately cut complex k_z plane to pass, as in reference 7, close to the point q_0 (choosing the $\pm$ in q_0

according to the sign of F) it is finally found that

$$M_{c+v+}(n)\cong(-i)\frac{\pi}{3}\exp\left(-\frac{\pi}{\sqrt{6}}\frac{P|q_0|^2}{|F|}\right). \quad (4.10)$$

For the tunneling between the $(-)$ bands it can be seen that it is obtained from the previous result simply by substituting $n+\frac{3}{4}$ for $n-\frac{3}{4}$ in the expression (4.7) for q_0.

Thus, expressing the matrix element P in terms of the reduced effective mass

$$m_r=(m_c^{-1}+|m_v|^{-1})^{-1}\cong m_c/2,$$

we have from (4.7), (4.10), and (3.5) for the transmission coefficient

$$D_{cv}^{\pm}(n)=|M_{c\pm v\pm}(n)|^2=(\pi/3)^2 \times\exp\{-\gamma[1+2(n\mp\tfrac{3}{4})\hbar\omega_r/\epsilon_g]\}, \quad (4.11)$$

where

$$\gamma=\tfrac{1}{2}\pi m_r^{\frac{1}{2}}\epsilon_g^{\frac{3}{2}}/\hbar|F| \quad (4.12)$$

and $\omega_r=eH/m_rc$. It must be remembered that for the $(+)$ bands $n=1, 2, 3, \cdots$; whereas for the $(-)$ bands $n=0, 1, 2, \cdots$.

Similarly, from (3.2) we find for the number of electrons per cm^3 sec that tunnel from a full light-hole $(\pm)$ valence band to an empty $(\pm)$ conduction band

$$w_{cv}^{\pm}(H)=\frac{1}{36}\frac{|F|}{\hbar}\frac{eH}{\hbar c}e^{-\gamma\frac{1}{2}}\operatorname{csch}\left(\gamma\frac{\hbar\omega_r}{\epsilon_g}\right) \times\exp\left(\pm\tfrac{1}{2}\gamma\frac{\hbar\omega_r}{\epsilon_g}\right), \quad (4.13)$$

with negligible error for all available magnetic-field strengths. For the total number of electrons tunneling from either light-hole valence band to the conduction bands we find

$$\frac{w_{cv}(H)}{w_{cv}}=\gamma\frac{\hbar\omega_r}{\epsilon_g}\operatorname{csch}\left(\gamma\frac{\hbar\omega_r}{\epsilon_g}\right)\cosh\left(\tfrac{1}{2}\gamma\frac{\hbar\omega_r}{\epsilon_g}\right). \quad (4.14)$$

Here, $w_{cv}=w_{cv}(H=0)$ is given by

$$w_{cv}=\frac{1}{18\pi}\frac{F^2}{\hbar^2}\frac{m_r^{\frac{1}{2}}}{\epsilon_g^{\frac{1}{2}}}e^{-\gamma}, \quad (4.15)$$

which is identical to Kane's[7] result.

Thus, the Zener current for InSb is a monotonically decreasing function of the longitudinal magnetic field. The reduction stems primarily from the increase in the effective energy gap due to the Landau quantization of the energy levels and the $\Delta n=0$ selection rule for the tunneling process. Similarly, Eq. (4.14) is a reliable estimate in spite of the fact that the wave functions used are good approximations to the true ones only for low quantum numbers n, since it is from these states that most of the tunneling proceeds.

The effect of the magnetic field on the tunneling current in an Esaki diode has been shown[4,5] to be given in its main features again by Eq. (4.14). The experimental results of Calawa *et al.*[1] are in good agreement with this formula.

It should be pointed out that the tunneling between the $(+)$ and $(-)$ bands has been neglected. This will not be examined in detail, but it is easy to see that it is justified in view of the fact that the matrix element Z_{v-c+} turns out to be much smaller than $Z_{v\pm c\pm}$ for all available magnetic fields and vanishes for $H=0$. In addition, the selection rule $\Delta n=0$ for the tunneling process $(v\pm\rightarrow c\mp)$ increases by $\hbar\omega_r$ the smallest energy gap over that of the corresponding minimum energy gap for the tunneling between the other bands. Thus, for high magnetic fields, the tunneling probability for such transitions is further reduced.

Finally, the neglect of the spin-orbit split-off band, with an energy separation $\Delta\approx 4\epsilon_g$, is justifiable for sufficiently low energies in the bands, where most of the tunneling occurs. Also the neglect of the tunneling from the heavy-hole band is justified in view of the critical dependence of the tunneling probability on the effective mass, Eq. (4.11).

APPENDIX

We seek solutions of $(\mathcal{H}-E)\psi=0$, where $\mathcal{H}$ is the total Hamiltonian in the presence of a magnetic field, in the form

$$\psi(\mathbf{r})=\textstyle\sum_\mu R_\mu(\mathbf{r})u_\mu(\mathbf{r}), \quad (A1)$$

with u_μ defined by (3.2). It is then easily found, by expanding $\mathbf{v}u_\mu=\sum_{\mu'}u_{\mu'}\mathbf{v}_{\mu'\mu}$, $\epsilon u_\mu=\sum_{\mu'}u_{\mu'}\epsilon_{\mu'\mu}$ and rearranging terms, that

$$(\mathcal{H}-E)\psi(\mathbf{r})=\sum_\mu u_\mu(\mathbf{r})\sum_{\mu'}(\mathfrak{L}_{\mu\mu'}-E\delta_{\mu\mu'})R_{\mu'}(\mathbf{r})=0, \quad (A2)$$

where the matrix operator $\mathfrak{L}_{\mu\mu'}$ is given by

$$\mathfrak{L}_{\mu\mu'}=\left(\frac{\boldsymbol{\pi}^2}{2m}+\mathcal{E}_\mu\right)\delta_{\mu\mu'}+\mathbf{v}_{\mu\mu'}\cdot\boldsymbol{\pi}+\epsilon_{\mu\mu'}, \quad (A3)$$

and $\boldsymbol{\pi}=\mathbf{p}+(e/c)\mathbf{A}$ is the kinetic momentum operator. Thus, every eigensolution $\{R_\mu(\mathbf{r})\}$ of

$$\sum_{\mu'}(\mathfrak{L}_{\mu\mu'}-E\delta_{\mu\mu'})R_{\mu'}(\mathbf{r})=0 \quad (A4)$$

provides an eigenfunction $\psi(\mathbf{r})$ through (A1) and with the same eigenvalue. (The completeness and linear independence of these eigenfunctions will not be discussed here.)

For the adopted vector potential depending only on x, the operators p_y, p_z commute with $\mathfrak{L}_{\mu\mu'}$ and thus we may seek solutions of (A4) in the form

$$R_\mu(\mathbf{r})=e^{ik_yy}e^{ik_zz}X_\mu(x+\hbar k_y/m\omega). \quad (A5)$$

In terms of the usual raising and lowering operators,

$\eta^{\pm}=[p_x \pm i(m\omega x+\hbar k_y)]/(2m\hbar\omega)^{\frac{1}{2}}$, X_μ are given by

$$EX_\mu=[\mathcal{E}_\mu+\hbar^2k_z^2/2m+(\eta^-\eta^+-\tfrac{1}{2})\hbar\omega]X_\mu + \sum_{\mu'}[\hbar k_z v_{\mu\mu'}{}^z+\epsilon_{\mu\mu'} + (2m\hbar\omega)^{\frac{1}{2}}(v_{\mu\mu'}{}^-\eta^+ + v_{\mu\mu'}{}^+\eta^-)]X_{\mu'}. \quad \text{(A6)}$$

For substances and a set of bands characterized by the selection rules (3.3) it is easily seen from the well known properties of the harmonic oscillator eigenfunctions $\Phi_n(x)$ that

$$X_\mu(x)=C_\mu(n)\Phi_{n-m(\mu)}(x), \quad \text{(A7)}$$

where $n-m(\mu)=0, 1, 2, \cdots$, and the coefficients C_μ and energy eigenvalues E are given by (3.4) and (3.5). Equations (A7), (A5), and (A1) prove Eqs. (3.1) and (3.4).

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Critical Concentrations in Magnetism

S. H. CHARAP
International Business Machines Corporation, Thomas J. Watson Research Center, Yorktown Heights, New York
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In the application of the Bethe-Peierls-Weiss method to dilute magnetism, Smart has exaggerated the interaction between a cluster and its surroundings by retaining the uniform molecular field. The calculation is improved by allowing the molecular field to vary from site to site on the first shell of the cluster, thereby taking into account the fact that this interaction is sensitive to the relative location of magnetic atoms in the first shell of the cluster and in the surrounding layer. For the three-dimensional lattices treated, the critical concentration is very nearly $2/z$, where z is the coordination number of the lattice.

THE theory of the behavior of a magnetic system (nearest-neighbor interactions only) when diluted by the substitution of a nonmagnetic component has been treated by a number of authors and the situation has recently been reviewed by Smart.[1] Of particular interest is the dependence of the ferromagnetic transition temperature (Curie point) on the concentration of the magnetic component p. Only on the molecular field picture does a finite Curie point exist for all finite values of p. More realistic models predict the occurrence of a critical concentration p_c below which ferromagnetism does not occur. The simplest of these is the "average coordination number" method of Sato *et al.*[2] This is a modification of the Bethe-Peierls-Weiss[3] (BPW) scheme in which the "first shell" of the cluster is assumed to have just pZ magnetic atoms, Z being the number of nearest-neighbor sites characteristic of the lattice. The result, $p_cZ=2$, is physically very suggestive, being just the concentration required for the magnetic atoms to make a linear chain in the crystal on the average. However, these authors[2] also point out that any extension of Bethe's method to the treatment of dilute ferromagnets must take into account all the possible concentration fluctuations which can occur in the system. If nearest-neighbor concentration fluctuations are permitted, then $p_c=(Z-1)^{-1}$. This result was obtained by Sato *et al.*[2] using the Takagi-Kikuchi[4] method and the Ising model, and also by Smart[1] in a direct extension of the BPW method using the classical spin approximation to the Heisenberg model of Brown and Luttinger.[5] In the latter calculation all possible kinds of clusters (magnetic atom populations) were considered with a uniform molecular field describing the interaction of "first shell" magnetic atoms with the remainder of the crystal.

The present work is an extension of Smart's treatment, motivated by the suspicion that the physical problem was inadequately represented because of the neglect of some of the longer range concentration fluctuations. To paraphrase Bethe,[6] the "force" tending to produce order at a given *cluster* will depend on the *occupation* of the *sites* in the immediate neighborhood of the *cluster* under consideration. In particular, with nearest-neighbor interactions alone, the uniform molecular field exaggerates the interaction between a cluster and its surroundings; since this is sensitive to the relative location of the magnetic atoms in the "first shell" of the cluster, and the surrounding layer or "second shell." Indeed, we find that the incorporation of fluctuations in the molecular field results in calculated values for p_c considerably larger than $(Z-1)^{-1}$ and quite close to those of Elliott *et al.*[7] and of Frisch *et al.*[8]

We assume that a "first shell" magnetic atom i is subject to a molecular field proportional to the number of magnetic neighbors n_i that it has outside the cluster (only lattices with no interactions within the first shell

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