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MINIBANDS IN SEMICONDUCTOR SUPERLATTICES MODELLED AS DIRAC COMBS (SIGNIFICANCE OF BAND NON-PARABOLICITY)

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A generalization of the Kronig-Penney problem is put forward with the potential energy $V(x) = \gamma \sum_j \delta(x - ja)$, $\gamma > 0$. A periodic multi-layer ...ABABABA... is considered: layers A of thickness a are intercalated between layers B of much smaller thickness. In this superlattice, A and B symbolize, respectively, narrow-gap semiconductor layers and barrier layers. The conduction band of the semiconductor A is defined by the dispersion function $E(\mathbf{k})$ which was derived in the Kane two-band theory. Owing to the non-zero value of the parameter γ, the electron energies inside the interval corresponding to the conduction band of the semiconductor A are organized in minibands separated by forbidden gaps. With $E(\mathbf{k})$ taken in the Kane form, the dispersion law $\mathcal{E} = E(\mathbf{k})$ is non-parabolic if E_g (the width of the forbidden gap of the semiconductor A) is finite. This non-parabolicity affects the positions and widths of the minibands. If E_g tends to infinity, the original Kronig-Penney problem is recovered. If E_g decreases, the density of the minibands increases.

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1 Introduction

The Kronig-Penney model [1, 2] belongs to text-book topics of the solid state theory. During the past decade, this model has become up to date owing to the great progress in fabrication of perfect semiconductor superlattices. For instance, the delta-doping proved to be a viable method for production of single-crystalline semiconductor samples with a very precise periodic modulation of the density of dopants [3–7]. In such a case, we may consider a given dispersion function $E(\mathbf{k})$ defining the conduction band of the pure semiconductor and add a periodic function $V(x)$ generated by the delta-doping with a spacing a. In our paper, we write $E(k)$ instead of $E(\mathbf{k})$, taking $k_y = k_z = 0$. (We omit the subscript x in k_x: $k = |\mathbf{k}|$ if $k_x > 0$ and $k = -|\mathbf{k}|$ if $k_x < 0$.) As long as a is much greater than the semiconductor lattice constant, the conduction band is split into narrow minibands separated by narrow gaps. Neglecting all interband matrix elements of $V(x)$, we may rely upon the one-band Schrödinger-Wannier equation [8] for the stationary envelope wave functions $\psi_{n,k}(x)$,

$$E(-i\partial/\partial x)\psi_{n,k}(x) + V(x)\psi_{n,k}(x) = E_n(k)\psi_{n,k}(x)\,. \quad (1)$$

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Here n means the miniband index. We define the function $V(x)$ as an array of delta-functions,

$$V(x) = \gamma \sum_j \delta(x - ja)\,, \tag{2}$$

with a constant $\gamma > 0$. The original Kronig-Penney problem concerns the approximation where $E(k)$ is taken as the quadratic function

$$E_{\mathrm{par}}(k) = \frac{\hbar^2 k^2}{2m}\,, \tag{3}$$

$m = \mathrm{const} > 0$. Then the dispersion law $\mathcal{E} = E(k)$ of the conduction electrons is parabolic.

The parabolic approximation need not always be satisfactory. In the present paper, we want to demonstrate that if the miniband index n is sufficiently high, the functions $E_n(k)$ can considerably depend on the non-parabolicity of the dispersion law $\mathcal{E} = E(k)$. Non-parabolicity effects were also studied in some of our previous papers [10–14]. In [10–13], we dealt with the Schrödinger-Wannier equation in which $V(x)$ was defined as a single delta-function, $V(x) = \gamma\delta(x)$. In [14], on the other hand, we have analyzed the resonance tunnelling in the case where $V(x) = \gamma[\delta(x - \frac{1}{2}a) + \delta(x + \frac{1}{2}a)]$. Moreover, we have also formulated a general theorem in [14] concerning the Schrödinger-Wannier equation with the function $V(x) = \sum_i \gamma_i \delta(x - x_i)$ involving arbitrary constants γ_i and x_i. This theorem, being valid for $\mathcal{E} > 0$, says that if we are interested in stationary solutions of the Schrödinger-Wannier equation with a quite *general* function $V(x)$ composed of delta-functions, we may use a general transformation directly converting the result derived at first with $E(k) \equiv E_{\mathrm{par}}(k)$ to the result concerning any other dispersion function $E(k)$. (We have only to presume that there is a one-to-one mapping between $E(k)$ and $E_{\mathrm{par}}(k)$.)

Following Flügge [9], we call the function defined by formula (2) the Dirac comb.

The function $E(k)$ is even, $E(k) = E(-k)$. We consider the lower boundary of the conduction band as the zero energy. Then $E(k) \geq 0$, $E(0) = \mathrm{d}E(k)/\mathrm{d}k|_{k=0} = 0$. We denote the effective mass of the conduction electrons as m:

$$\frac{1}{\hbar^2}\frac{\mathrm{d}^2 E(k)}{\mathrm{d}k^2}\bigg|_{k=0} = \frac{1}{m} > 0\,.$$

In our calculations, we will confine ourselves to an interval $(0, \bar{E})$ of electron energies, assuming that $\bar{E}$ lies somewhere in the central part of the conduction band described by the function $E(k)$. We require that the equation $\mathcal{E} = E(k)$ has only one root $k(\mathcal{E})$ in the interval $(0, \bar{E})$ and that $\mathrm{d}E(k)/\mathrm{d}k > 0$ for $k > 0$ if $0 < E(k) < \bar{E}$.

As an illustration, we juxtapose (in Section 3) the original Kronig-Penney result valid for the quadratic dispersion function (3) with the result obtained with the Kane dispersion function

$$E_{\mathrm{Kane}}(k) = \frac{E_{\mathrm{g}}}{2}\left[\left(1 + \frac{2\hbar^2 k^2}{m E_{\mathrm{g}}}\right)^{1/2} - 1\right]. \tag{4}$$

($E_{\mathrm{g}} > 0$ is the width of the forbidden gap.) The Kane function is particularly important in the theory of narrow-gap semiconductors [15–19]. Clearly, $E_{\mathrm{Kane}}(k) \to E_{\mathrm{par}}(k)$ if $E_{\mathrm{g}} \to \infty$.

2 General theory

The Hamiltonian $H(x) = E(-\mathrm{i}\partial/\partial x) + \gamma \sum_j \delta(x - ja)$ is invariant with respect to any translation $x' = x - ja$, $j = 0, \pm 1, \dots$, so we may write its eigen-functions in the Bloch form

$$\psi_{n,k}(x) = u_{n,k}(x) \exp(\mathrm{i}kx)\,, \tag{5}$$

where $u_{n,k}(x+a) = u_{n,k}(x)$ and $-\pi/a < k \leq \pi/a$. The wave functions have to be continuous at the positions $x_j = ja$ of the deltas, so we write

$$\psi_{n,k}(x)|_{x_j+0} = \psi_{n,k}(x)|_{x_j-0} = \psi_{n,k}(x_j) \tag{6}$$

and

$$\psi_{n,k}(a) = \exp(\mathrm{i}ka)\psi_{n,k}(0)\,. \tag{7}$$

The values $\partial^s \psi_{n,k}(x)/\partial x^s|_{x_j+0}$ and $\partial^s \psi_{n,k}(x)/\partial x^s|_{x_j-0}$ (for any chosen value of $s = 1, 2, \dots$) have to satisfy the equalities

$$\partial^s \psi_{n,k}(x)/\partial x^s|_{x=a+0} = \exp(\mathrm{i}ka)\partial^s \psi_{n,k}(x)/\partial x^s|_{x=+0}\,, \tag{8$^+$}$$

$$\partial^s \psi_{n,k}(x)/\partial x^s|_{x=a-0} = \exp(\mathrm{i}ka)\partial^s \psi_{n,k}(x)/\partial x^s|_{x=-0}\,. \tag{8$^-$}$$

Since we have chosen $\gamma > 0$, all the eigen-energies $E_n(k)$ are positive. Let us take into account some value $\mathcal{E} > 0$ and write

$$\psi_{n,k}(x) = \exp(\mathrm{i}\kappa x) + C \exp(-\mathrm{i}\kappa x)$$

for $0 \leq x < a$, with $\kappa > 0$ determined by the equation

$$\mathcal{E} = E(\kappa)\,. \tag{9}$$

Because $\mathcal{E}$ is equal to one of possible values of $E_n(k)$, the parameter κ and the coefficient C depend on n and k. Our main intent is to clarify the structure of the minibands. Therefore, we may put away the formal question of the normalization of the eigen-functions $\psi_{n,k}(x)$. In regard to equations (6) and (7), we can at once write down the equation

$$1 + C = \exp(-\mathrm{i}ka)\,[\exp(\mathrm{i}\kappa a) + C \exp(-\mathrm{i}\kappa a)]\,. \tag{10}$$

However, we can also formulate a relation between right-hand and left-hand derivatives of $\psi_{n,k}(x)$ at $x = 0$. For this purpose, we define the group velocity $v(k) = \hbar^{-1}\partial E(k)/\partial k$ and, substituting $-\mathrm{i}\partial/\partial x$ for k, the operator $v(-\mathrm{i}\partial/\partial x)$. In [10], we have proved by the Fourier analysis (having treated the single delta-barrier case, but a generalization allowing the presence of an arbitrary number of delta-barriers was presented later on in [14]), the equality

$$-\mathrm{i}\hbar\left[v(-\mathrm{i}\partial/\partial x)\psi_{n,k}(x)|_{x=+0} - v(-\mathrm{i}\partial/\partial x)\psi_{n,k}(x)|_{x=-0}\right] + 2\gamma\psi_{n,k}(0) = 0\,.$$

From this equality, respecting eqs. (8^+) and (8^-), we derive the equation

$$-\,\mathrm{i}\hbar\,\{v(\kappa)+C\,v(-\kappa)\;-\;\exp(-\mathrm{i}ka)[v(\kappa)\exp(\mathrm{i}\kappa a)+C\,v(-\kappa)\exp(-\mathrm{i}\kappa a)]\}\\ +\;2\gamma\,(1+C)=0\,.$$

This equation, as $v(-\kappa) = -\,v(\kappa)$, can be rewritten in the form

$$-\,\mathrm{i}\hbar\,v(\kappa)\left[1-C\;-\;\exp(-\mathrm{i}ka)[\exp(\mathrm{i}\kappa a)-C\exp(-\mathrm{i}\kappa a)]\right]+\;2\gamma\,(1+C)=0\,. \qquad (11)$$

Equations (10) and (11) give the equation

$$\cos(ka)=\cos(\kappa a)+\hbar\gamma\,\frac{\sin(\kappa a)}{v(\kappa)}\,. \qquad (12)$$

In particular, if $E(k)\equiv E_{\mathrm{par}}(k)$, equation (12) is reduced to the well-known Kronig-Penney equation

$$\cos(ka)=\cos(\kappa a)+m\gamma\,\frac{\sin(\kappa a)}{\kappa}\,. \qquad (12^{\mathrm{par}})$$

The r. h. sides of eqs. (12) and (12^{par}) are unique functions of the variable κ. Using the dimensionless variable

$$\chi=\kappa a\,, \qquad (13)$$

we write

$$Z(\kappa)\;\equiv\;\mathcal{A}(\chi,\kappa)=\cos(\chi)+\hbar\gamma\,\frac{\sin(\chi)}{v(\kappa)}\,, \qquad (14)$$

$$Z_{\mathrm{par}}(\kappa)\;\equiv\;\mathcal{A}_{\mathrm{par}}(\chi,\kappa)=\cos(\chi)+m\gamma\,\frac{\sin(\chi)}{\kappa}\,. \qquad (14^{\mathrm{par}})$$

The identity

$$\mathcal{A}(\chi,\kappa)=\mathcal{A}_{\mathrm{par}}(\chi,mv(\kappa)/\hbar) \qquad (15)$$

manifests our theorem formulated in [14].

3 Results for $E(k)\equiv E_{\mathrm{par}}(k)$ and for $E(k)\equiv E_{\mathrm{Kane}}(k)$

We define the dimensionless parameter

$$\beta=\frac{ma}{\hbar^2}\,\gamma \qquad (16)$$

and the dimensionless function

$$\Phi(\chi)=\frac{ma}{\hbar}\,v(\kappa)\,. \qquad (17)$$

Then equation (12) reads

$$\cos(ka)=\cos(\chi)+\beta\,\frac{\sin(\chi)}{\Phi(\chi)}\,. \qquad (18)$$

Recall that $v_{\mathrm{par}}(\kappa)=\hbar\kappa/m$. Thus $\Phi_{\mathrm{par}}(\chi)=\chi$.

Moreover, considering the Kane dispersion function (4), we define the dimensionless non-parabolicity parameter

$$\eta_{\mathrm{g}}=\frac{ma^2}{\hbar^2}\,E_{\mathrm{g}}\,. \qquad (19)$$

In order to typify a realistic value of η_{g} for conduction electrons in a semiconductor superlattice, let us consider the parameters for GaAs at 300 K: $E_{\mathrm{g}}\approx 1.43$ eV and $m/m_0=0.07$ [20]. Then, with the superlattice constant $a\approx 28$ nm, we obtain $\eta_{\mathrm{g}}\approx 1000$. For

$$v_{\mathrm{Kane}}(\kappa)=\frac{\hbar\kappa}{m}\left(1+\frac{2\hbar^2\kappa^2}{mE_{\mathrm{g}}}\right)^{-1/2}, \qquad (20)$$

we obtain the function

$$\Phi_{\mathrm{Kane}}(\chi)=\chi\left(1+\frac{2\chi^2}{\eta_{\mathrm{g}}}\right)^{-1/2}. \qquad (21)$$

Clearly, $\Phi_{\mathrm{Kane}}(\chi)$ goes over into $\Phi_{\mathrm{par}}(\chi)$ if $\eta_{\mathrm{g}}\to\infty$. The r. h. side of eq. (18),

$$\zeta(\chi)\;\equiv\;Z(\chi/a)\;\equiv\;\mathcal{A}(\chi,\chi/a)=\cos(\chi)+\beta\,\frac{\sin(\chi)}{\Phi(\chi)}\,, \qquad (22)$$

in the two cases in question is specified as follows:

$$\zeta_{\mathrm{par}}(\chi)=\cos(\chi)+\beta\,\frac{\sin(\chi)}{\chi}\,, \qquad (22^{\mathrm{par}})$$

$$\zeta_{\mathrm{Kane}}(\chi)=\cos(\chi)+\beta\left(1+\frac{2\chi^2}{\eta_{\mathrm{g}}}\right)^{1/2}\frac{\sin(\chi)}{\chi}\,. \qquad (22^{\mathrm{Kane}})$$

The functions $\zeta_{\mathrm{par}}(\chi)$ and $\zeta_{\mathrm{Kane}}(\chi)$ are shown in Fig. 1 for $\beta=10$ and for $\eta_{\mathrm{g}}=20$. The shaded regions in Fig. 1 correspond to the allowed values of $\chi=\kappa a$.

According to eq. (18), it is sufficient to take the values of k from the positive half (including the zero point) of the first Brillouin zone: $0\le k\le\pi/a$. Having in mind the nth shaded region in Fig. 1, we write $\chi\equiv\chi_n(ka)$, since the roots $\chi\equiv\chi_n$ of eq. (18) depend on the dimensionless variable ka. Clearly, the limes superior of χ_n is equal to $\chi_n(\pi)=n\pi$ for odd n and to $\chi_n(0)=n\pi$ for even n. If n is odd, the limes inferior of χ_n, being equal to $\chi_n(0)$, is to be calculated from the equation $\zeta(\chi_n(0))=1$. On the other hand, if n is even, then the limes inferior of χ_n, being equal to $\chi_n(\pi)$, fulfills the equation $\zeta(\chi_n(\pi))=-\,1$. To avoid any ambiguity, we postulate the identification of $\chi_n(0)$ if n is odd (of $\chi_n(\pi)$ if n is even) with the nearest root lying on the left to the value $n\pi$.

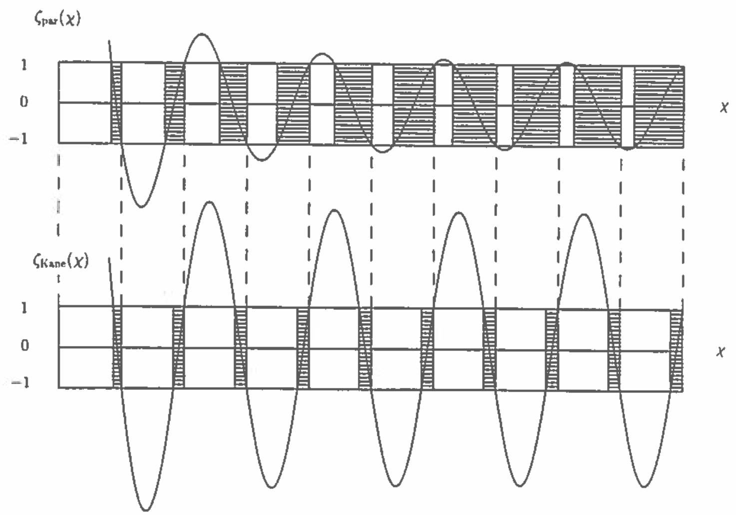

Fig. 1. Illustration of the Kronig-Penney-type calculation of the minibands. The cross-sections of the horizontal straight lines $\cos(ka) = $ const with the corresponding oscillating curve define the dependences $\kappa = \kappa_n(k)$ $(\chi_n = \kappa_n a)$. The dashed vertical straight lines correspond to $\chi = \pi n$, $n = 0, 1, 2, \ldots$ Respectively, the upper part and the lower part of the figure correspond to the values $\beta = 10$, $\eta_g = \infty$ and $\beta = 10$, $\eta_g = 20$.

With this definition of the miniband number n, we may consider the roots of the equations $\cos(ka) = \zeta_{\rm par}(\chi)$ and $\cos(ka) = \zeta_{\rm Kane}(\chi)$ as uniquely defined functions of the variable ka; we denote them, respectively, as $\chi_{{\rm par}\ n}(ka)$ and $\chi_{{\rm Kane}\ n}(ka)$.

In analogy to relation (19), we define the dimensionless energy functions

$$\eta_{\rm par}(\chi) = \frac{\chi^2}{2}\,, \tag{23$^{\rm par}$}$$

$$\eta_{\rm Kane}(\chi) = \frac{\eta_g}{2}\left[(1 + 2\chi^2/\eta_g)^{1/2} - 1\right]. \tag{23$^{\rm Kane}$}$$

When replacing χ by $\chi_{{\rm par}\ n}(ka)$ and $\chi_{{\rm Kane}\ n}(ka)$ in the corresponding functions $\eta_{\rm par}(\chi)$ and $\eta_{\rm Kane}(\chi)$, we obtain the dispersion functions

$$e_{{\rm par}\ n}(ka) \equiv \mathcal{E}_{\rm par}(\chi_{{\rm par}\ n}(ka)) \tag{24$^{\rm par}$}$$

and

$$e_{{\rm Kane}\ n}(ka) \equiv \mathcal{E}_{\rm Kane}(\chi_{{\rm Kane}\ n}(ka)) \tag{24$^{\rm Kane}$}$$

for the minibands.

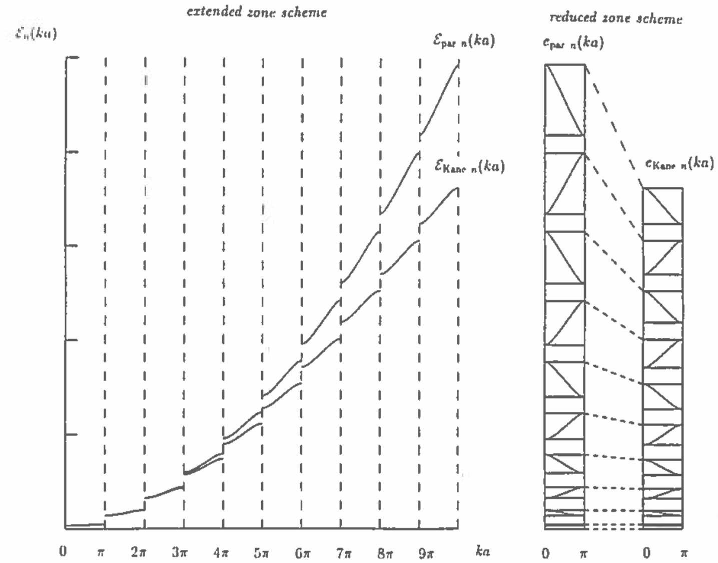

Fig. 2. The plot (in arbitrary units) of the energy *versus* wave vector obtained from calculations with $\beta = 10$, $\eta_g = 1000$. The r. h. part of the figure exhibits the miniband dispersion functions in the reduced BZ scheme. The 'wavelets' in the higher (in the lower) column show the functions $e_{{\rm par}\ n}(ka)$ (the functions $e_{{\rm Kane}\ n}(ka)$). The l. h. part of the figure exhibits these miniband dispersion functions in the extended BZ scheme. In the latter, the 'wavelets' due to the minibands with even indices are mirror images (with respect to vertical axes) of the corresponding 'wavelets' in the reduced BZ scheme.

These functions are shown in Fig. 2. To exemplify that the value $\beta \approx 10$ for $\eta_g \approx 1000$ is acceptable, let us replace the delta-function pseudopotential $\gamma\delta(x)$ by a rectangular barrier of height V_0 and width w so that $\gamma \approx V_0 w$. Then, from formulae (16) and (19), we obtain the relationship

$$\beta \approx \frac{w}{a}\,\frac{V_0}{E_g}\,\eta_g\,. \tag{25}$$

When taking, for instance, $w \approx a/20$, $V_0 \approx E_g/5$, we find that $\beta \approx 10$ for $\eta_g \approx 1000$. (We have used another value of η_g in Fig. 1 in order to make this figure more expressive.) The r. h. part of Fig. 2 manifests the reduced Brillouin zone scheme. In the l. h. part of Fig. 2, we have plotted the miniband functions within the framework of the extended Brillouin zone scheme as well. In the extended Brillouin zone scheme, the nth miniband corresponds to the interval $(n-1)\pi \le ka \le n\pi$. The upper curve (the lower curve) in this interval shows the function $e_{{\rm par}\ n}(ka - (n-1)\pi)$

(the function $e_{\text{Kane}\ n}(ka-(n-1)\pi)$) if n is odd and the function $e_{\text{par}\ n}(n\pi - ka)$ (the function $e_{\text{Kane}\ n}(n\pi - ka)$) if n is even. The two columns in r. h. part of the figure exhibit the reduced Brillouin zone scheme: the functions $e_{\text{par}\ n}(ka)$ and $e_{\text{Kane}\ n}(ka)$ are shown in the higher and in the lower column, respectively ($n = 1, 2, \ldots$).

4 Concluding remarks

The generalization of the Kronig-Penney problem, as we have presented it in this paper, has resulted from our former derivation [10, 14] of the conditions which had to be posed on the eigen-functions $\psi_{\mathcal{E}}(\mathbf{r})$ of the Schrödinger-Wannier equation with $V(x) = \sum_j \gamma_j \delta(x - x_j)$. These conditions were derived under the assumption that $\mathcal{E} > 0$. Although the model of the Dirac comb is certainly an overidealization if we have in mind actually existing semiconductor superlattices, our calculations have confirmed, in a simple quantitative way, that the band non-parabolicity can very noticeably affect not only the positions but also the shapes of the miniband dispersion functions $e_n(ka) = (ma^2/\hbar^2)\, E_n(k)$.

It is not surprising that the curves $\mathcal{E} = E_{\text{Kane}\ n}(k)$ are shifted downwards against the curves $\mathcal{E} = E_{\text{par}\ n}(k)$. The shift for $k = \pi/a$ (in the reduced Brillouin zone scheme) is equal to

$$E_{\text{par}\ n}(\pi/a) - E_{\text{Kane}\ n}(\pi/a) = E_{\text{par}}(n\pi/a) - E_{\text{Kane}}(n\pi/a)\,. \tag{26}$$

Formula (26) follows from the identity

$$E_n(\pi/a) = E(n\pi/a)\,. \tag{27}$$

On account of eq. (27), it is natural to define a function $g^{\text{mb}}(n)$ of the discrete variable n interpreted as the density of minibands:

$$g^{\text{mb}}(n) = \frac{a}{\pi}\,\frac{1}{\partial E(k)/\partial k}\bigg|_{k=\pi n/a}\,. \tag{28}$$

For the dispersion laws dealt with in this paper, we have got the functions

$$g^{\text{mb}}_{\text{par}}(n) = \frac{ma^2}{\hbar^2}\,\frac{1}{\pi^2 n} \tag{28$^{\text{par}}$}$$

and

$$g^{\text{mb}}(n) = \frac{ma^2}{\hbar^2}\,\frac{\sqrt{1+2\pi^2 n^2/\eta_{\text{g}}}}{\pi^2 n}\,. \tag{28$^{\text{Kane}}$}$$

Clearly, the asymptotic values $g^{\text{mb}}_{\text{Kane}}(\infty)$ and $g^{\text{mb}}_{\text{par}}(\infty)$ are qualitatively different:

$$g^{\text{mb}}_{\text{par}}(\infty) = 0\,, \tag{29$^{\text{par}}$}$$

$$g^{\text{mb}}_{\text{Kane}}(\infty) = \frac{ma^2}{\hbar^2}\,\frac{1}{\pi}\left(\frac{2}{\eta_{\text{g}}}\right)^{1/2}. \tag{29$^{\text{Kane}}$}$$

This difference is, of course, due to the fact that $E_{\text{par}}(k) \sim k^2$ but $E_{\text{Kane}}(k) \sim k$ for $k \to \infty$.

Our final remark concerns forbidden gaps between the minibands. Let ΔE^{mb}_n be the width of the allowed nth miniband corresponding to the dispersion law $\mathcal{E} = E(k)$ and let ΔE^{fb}_n be the width of the forbidden gap just touching the nth allowed miniband from below. Then we introduce the ratio

$$f^{\text{empty}}(n) = \frac{\Delta E^{\text{fb}}_n}{\Delta E^{\text{fb}}_n + \Delta E^{\text{mb}}_n} \tag{30}$$

determining the percentage of forbidden energy values in the interval of the width

$$\Delta E^{\text{fb}}_n + \Delta E^{\text{mb}}_n = E(n\pi/a) - E((n-1)\pi/a)\,. \tag{31}$$

centred in the value $\frac{1}{2}[E(n\pi/a) + E((n-1)\pi/a)]$. From obvious reasons, we call $f^{\text{empty}}(n)$ the factor of emptiness of the energy spectrum near the nth miniband. When using the dimensionless functions $e_{\text{par}\ n}(ka)$ and $e_{\text{Kane}\ n}(ka)$ (defined in the reduced Brillouin zone scheme, cf. formulae (24$^{\text{par}}$), (24$^{\text{Kane}}$)), we can write, respectively, the factor of emptiness $f^{\text{empty}}_{\text{par}}(n)$, $f^{\text{empty}}_{\text{Kane}}(n)$ as follows.
For odd n:

$$f^{\text{empty}}_{\text{par}}(n) = \frac{e_{\text{par}\ n}(0) - e_{\text{par}\ n-1}(0)}{e_{\text{par}\ n}(\pi) - e_{\text{par}\ n-1}(0)}\,,$$

$$f^{\text{empty}}_{\text{Kane}}(n) = \frac{e_{\text{Kane}\ n}(0) - e_{\text{Kane}\ n-1}(0)}{e_{\text{Kane}\ n}(\pi) - e_{\text{Kane}\ n-1}(0)}\,.$$

For even n:

$$f^{\text{empty}}_{\text{par}}(n) = \frac{e_{\text{par}\ n}(\pi) - e_{\text{par}\ n-1}(\pi)}{e_{\text{par}\ n}(0) - e_{\text{par}\ n-1}(\pi)}\,,$$

$$f^{\text{empty}}_{\text{Kane}}(n) = \frac{e_{\text{Kane}\ n}(\pi) - e_{\text{Kane}\ n-1}(\pi)}{e_{\text{Kane}\ n}(0) - e_{\text{Kane}\ n-1}(\pi)}\,.$$

These functions of the integer variable n are plotted in Fig. 3. Extending formally the energy interval $(0, \tilde{E})$ to infinity, we may say that the asymptotic value of $f^{\text{empty}}(n)$ for $E(k) \equiv E_{\text{par}}(k)$ is equal to zero,

$$f^{\text{empty}}_{\text{par}}(\infty) = 0\,. \tag{32$^{\text{par}}$}$$

To calculate the asymptotic value $f^{\text{empty}}_{\text{Kane}}(\infty)$, let us assume, for instance, that n is odd. With $n = 2p+1$ (where p runs over non-negative integer values), when taking $p \to \infty$, we obtain the equation

$$1 \approx \cos\left[\chi_{\text{Kane}\ 2p+1}(0)\right] + \beta\left(\frac{2}{\eta_{\text{g}}}\right)^{1/2} \sin\left[\chi_{\text{Kane}\ 2p+1}(0)\right]\,,$$

from which

$$\chi_{\text{Kane}\ 2p+1}(0) \approx 2p\,\pi + 2\arctan\left[\beta\left(\frac{2}{\eta_{\text{g}}}\right)^{1/2}\right].$$

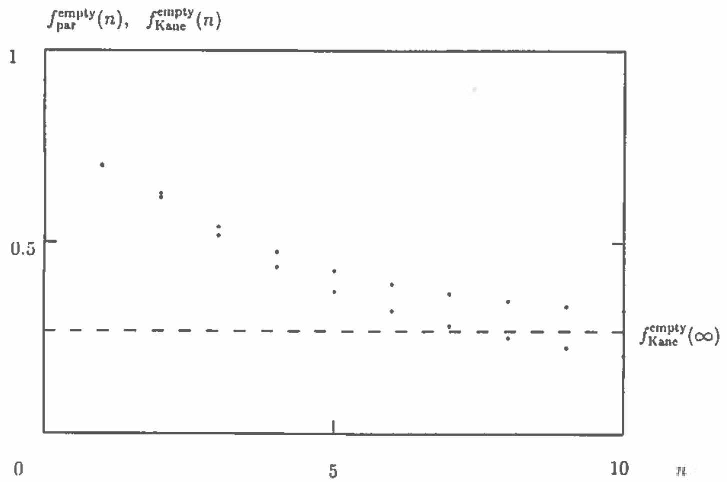

Fig. 3. The illustration of the 'emptiness' of the miniband spectra. In each pair of the points for any value of n, the lower (upper) point corresponds to the case when $E(k) \equiv E_{\rm par}(k)$ (when $E(k) \equiv E_{\rm Kane}(k)$) with $\beta = 10$, $\eta_{\rm g} = 1000$. The dashed line corresponds to the asymptotic value $f_{\rm Kane}^{\rm empty}(\infty) = (2/\pi)\arctan[(2/\eta_{\rm g})^{1/2}]$.

We could also take even values of n, obtaining the same value $f_{\rm Kane}^{\rm empty}(\infty)$. In the calculation of $\chi_{{\rm Kane}\ 2p}(\pi)$, we may employ the equation

$$-1 \approx \cos\left[\chi_{{\rm Kane}\ 2p}(\pi)\right] + \beta\left(\frac{2}{\eta_{\rm g}}\right)^{1/2} \sin\left[\chi_{{\rm Kane}\ 2p}(\pi)\right],$$

from which

$$\chi_{{\rm Kane}\ 2p}(\pi) \approx (2p-1)\,\pi + 2\arctan\left[\beta\left(\frac{2}{\eta_{\rm g}}\right)^{1/2}\right].$$

Asymptotically

$$e_{\rm Kane}(\chi) \approx \frac{\eta_{\rm g}}{2}\left[\left(\frac{2}{\eta_{\rm g}}\right)^{1/2}\chi - 1 + \mathcal{O}(1/\chi)\right].$$

Hence, with $n = 2p+1$, we obtain the result

$$f_{\rm Kane}^{\rm empty}(\infty) = \lim_{p\to\infty} \frac{e_{{\rm Kane}\ 2p+1}(0) - e_{{\rm Kane}\ 2p}(0)}{e_{{\rm Kane}\ 2p+1}(\pi) - e_{{\rm Kane}\ 2p}(0)} =$$
$$\frac{\chi_{{\rm Kane}\ 2p+1}(0) - \chi_{{\rm Kane}\ 2p}(0)}{\chi_{{\rm Kane}\ 2p+1}(\pi) - \chi_{{\rm Kane}\ 2p}(0)} = \frac{2}{\pi}\arctan\left[\left(\frac{2}{\eta_{\rm g}}\right)^{1/2}\right], \quad (32^{\rm Kane})$$

as $\chi_{{\rm Kane}\ 2p}(0) = 2p\pi$ and $\chi_{{\rm Kane}\ 2p+1}(\pi) = (2p+1)\pi$.

When comparing formulae ($32^{\rm par}$) and ($32^{\rm Kane}$) (or when looking at Figs. 2 and 3), one sees that the spectrum of the minibands is much 'emptier' for $E(k) \equiv E_{\rm Kane}(k)$ than for $E(k) \equiv E_{\rm par}(k)$. The striking distinction consisting in the non-zero value of $f_{\rm Kane}^{\rm empty}(\infty)$ and the zero value of $f_{\rm par}^{\rm empty}(\infty)$ is attributed to the distinction in the asymptotic behaviour (for $k \to \infty$) of the corresponding dispersion functions. (Indeed, for $k \to \infty$, we may deem the dependence $E_{\rm Kane}(k) \sim k$ as qualitatively different from the dependence $E_{\rm par}(k) \sim k^2$.)

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