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KANE OSCILLATOR IN THE QUASI-CLASSICAL APPROXIMATION

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The 1D Kane oscillator is analysed. It is defined by the Schrödinger-Wannier equation in which the potential-energy term represents the zero-centred quadratic well and in which the 'kinetic-energy' term is chosen as an operator corresponding to the conduction-electron dispersion function of the Kane two-band theory. The author considers the approximate form of the Kane function for the conduction band well-known in the theory of narrow-gap semiconductors. Employing the momentum representation, he calculates the eigen-energies of the electrons in frame of the WKB approach. The eigen-energies are roots of a transcendental equation involving the complete elliptic integrals of the first and second kind. The author presents a detailed discussion of the dependence of the eigen-energies of the electrons on the Kane nonparabolicity of the conduction band.

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1 Introduction

Recently Gashimzade and Babaev published a short paper [1] describing a quantum dot as a Kane oscillator. They focused attention on the Kane eight-band model referring to results derived by Darnhofer and Rössler [2]. In our present paper, we will direct attention on the Kane two-band model. We will not treat a dot, but a thin film, modelling the perpendicular confining potential by the quadratic function

$$V(z) = \frac{1}{2}\, K z^2 \quad (K > 0)\,. \tag{1}$$

This function (meaning, within the framework of the theory of envelope wave functions, the perpendicular profile of the lower boundary of the conduction band) was deemed reasonable by some theorists from the very beginning of the theory of the 'thin-film quantization', although the majority of investigators, when having directed attention to a semiconductor thin film, preferred to use another model—the Sommerfeld model with $V(z) = 0$ and with boundary conditions requiring zero values of the envelope functions of the conduction electrons at the surfaces of the film [3]. Nevertheless, the model with the function $V(z)$ defined by expression (1) has proved to

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be advantageous in some theories. For instance, it allowed to accomplish (whilst the Sommerfeld model did not) the complete analytical calculation of the one-electron propagator concerning a thin film in a *non-perpendicular* constant magnetic field $\mathbf{B}$. (The Sommerfeld model implies that conduction electrons bounce off elastically from the film surfaces like balls. Even if the quantum mechanics of these electrons can be formulated by means of Feynman's path-integral theory, the classical trajectories—which are the basic attribute of the Feynman theory with quadratic Lagrangians—are extremely intricate in the case of a general orientation of $\mathbf{B}$. Therefore, it is difficult to calculate the one-electron propagator. This difficulty is circumvented if $V(z)$ is defined as a quadratic function.)

However, the quadratic confinement model affords an opportunity to discuss interesting aspects of the solid-state theory even if $\mathbf{B} = 0$ and we will only deal with such a case.

If the value of K in function (1) is high, the conduction electrons are confined in a narrow 'layer', i.e. their perpendicular positional uncertainty, Δz, is small. But then, their momentum uncertainty, $\Delta p_z \approx \hbar/\Delta z$, is considerable. This indicates that if we consider the one-electron Hamiltonian with the potential energy $\frac{1}{2}Kz^2$, the lowest perpendicular energy eigen-value may be high and, correspondingly, the distances between perpendicular energy eigen-values may also be large enough. Then, even if we may approximate, with sufficiently low values of K, the dispersion function of the conduction electrons (in the perpendicular direction), $E(k_z)$, by the usual quadratic function $\hbar^2 k_z^2/(2m)$, this possibility ceases to be acceptable with such values of K when $V(z)$ may model nanometre confinements. In such a case, a good theory has to reckon with the nonparabolicity of the dispersion law $E = E(\mathbf{k})$, especially if we consider *narrow-gap* semiconductor thin films. The dispersion function $E(\mathbf{k})$ of the conduction electrons in narrow-gap semiconductors can well be approximated—at least in an interval $(0, \tilde{E})$ where $\tilde{E} > 0$ is a value comparable with the width $E_{\rm g} > 0$ of the forbidden energy gap—by the Kane function [4–8]

$$E_{\rm Kane}(\mathbf{k}) = \frac{E_g}{2}\left[\left(1 + \frac{2\hbar^2 k^2}{mE_g}\right)^{1/2} - 1\right]. \tag{2}$$

Here $k^2 = |\mathbf{k}|^2$. Since the direct-gap semiconductors are cubic, the effective mass $m > 0$ of the conduction electrons may be considered as a scalar,

$$\frac{1}{m} = \frac{1}{\hbar^2}\left.\frac{\partial^2 E_{\rm Kane}(\mathbf{k})}{\partial k^2}\right|_{k=0}.$$

Expression (2) is a simplified modification of the Kane function which has followed from his two-band perturbation theory. If $m_0 > 0$ is the factual electron mass, the dispersion function of conduction electrons according to the $\mathbf{k}.\mathbf{p}$-approximation [9] would, in the two-band theory, be equal to

$$E_{\rm k.p}(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_0} + \frac{E_{\rm g}}{2}\left\{\left[1 + \frac{2\hbar^2}{E_{\rm g}}\left(\frac{1}{m} - \frac{1}{m_0}\right)k^2\right]^{1/2} - 1\right\}.$$

However, in some semiconductors, the effective mass m is much smaller than m_0. (A notable example is InSb where the value of m is by two orders of magnitude smaller than m_0.) When neglecting $1/m_0$ against $1/m$ and omitting the term $\hbar^2 k^2/(2m_0)$, we find that $E_{\rm k.p}(\mathbf{k})$ is approximately equal to expression (2).

Throughout the present paper, we take $k_x = k_y = 0$. Thus we will analyse a 1D quantum-mechanical problem defined, in the z-representation, by the Schrödinger-Wannier equation

$$\left[E_{\mathrm{Kane}}\left(-\,\mathrm{i}\frac{\partial}{\partial z}\right) + \frac{1}{2}\,Kz^2\right]\psi_n(z) = E_n\psi_n(z)\,. \tag{3}$$

Here $E_{\mathrm{Kane}}(-\,\mathrm{i}\partial/\partial z)$ is the differential operator obtained from the function $E_{\mathrm{Kane}}(k_z)$ by substituting $-\,\mathrm{i}\partial/\partial z$ for k_z. The eigen-energies $E_n > 0$ form a discrete spectrum and are non-degenerated, $n = 0, 1, 2, \ldots$ The eigen-functions may be considered as real functions. Formally, equation (2) is a one-band equation, concerning the conduction band only. The influence of the valence band has been respected in the derivation of the Kane function. The proximity of the valence band to the conduction band causes the nonparabolicity of the dispersion law of the conduction electrons. (Indeed, only if $E_{\mathrm{g}} \to \infty$, the Kane function is reduced to the quadratic function $\hbar^2k^2/(2m)$.) Regarding the dynamics of the conduction electrons as essentially separated from the dynamics of the holes, we will solve equation (3) in the quasi-classical approximation.

The standard outline of the quasi-classical approximation (or, synonymously saying, the WKB approximation) can be found in many quantum-mechanical monographs. (Cf. e.g. [10].)

2 Solution of the problem

In compendia on quantum mechanics, the quasi-classical approximation was described, as a rule, in the position representation. In our paper, on the other hand, we will employ the momentum representation, with the Fourier transform

$$\phi_n(k_z) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\mathrm{d}z\,\exp(-\,\mathrm{i}k_z z)\psi_n(z)$$

in the role of the eigen-function. Then equation (3) is transformed into the equation

$$-\,\frac{K}{2}\,\frac{\partial^2\phi_n(k_z)}{\partial k_z^2} + E_{\mathrm{Kane}}(k_z)\phi_n(k_z) = E_n\phi_n(k_z)\,. \tag{4}$$

Formally taken, we can reinterpret this equation as if it were the Schrödinger equation in a fictitious position representation. We propose to use

$$\mu = \frac{\hbar^2 K}{E_{\mathrm{g}}^2} > 0$$

as a fictitious mass and

$$\xi = \frac{\hbar k_z}{\sqrt{\mu K}} = \frac{E_{\mathrm{g}}k_z}{K}$$

as a fictitious position variable. With the wave function

$$\tilde{\psi}_n(\xi) = \phi_n(\sqrt{\mu K}\,\xi/\hbar) = \phi_n(K\xi/E_{\mathrm{g}})$$

and the 'potential energy'

$$\tilde{V}(\xi) = E_{\mathrm{Kane}}(\sqrt{\mu K}\,\xi/\hbar) = E_{\mathrm{Kane}}(K\xi/E_{\mathrm{g}})\,,$$

equation (4) goes over into the 1D Schrödinger equation

$$-\frac{\hbar^2}{2\mu}\,\frac{\partial^2\tilde{\psi}_n(\xi)}{\partial\xi^2}+\tilde{V}(\xi)\tilde{\psi}_n(\xi)=E_n\tilde{\psi}_n(\xi)\,,$$

i.e.

$$-\frac{\hbar^2}{2\mu}\,\frac{\partial^2\tilde{\psi}_n(\xi)}{\partial\xi^2}\;+\;\frac{E_g}{2}\left[\sqrt{1\;+\;\frac{2\mu K}{mE_g}\,\xi^2}\;-\;1\right]\tilde{\psi}_n(\xi)=E_n\tilde{\psi}_n(\xi)\,. \tag{5}$$

To the best of our knowledge, this equation was not solved in an exact analytical way yet. The eigen-functions of this equation are surely not expressible in terms of elementary functions and we doubt whether there exists a simple possibility to express them in terms of known special functions.

Fortunately, we can solve equation (5) approximately by employing the WKB technique which reputably has lead to satisfactory results in the theory of semiconductor quantum films, wires and dots. Moreover, the WKB method is universal in the sense that it is equally suitable for a broad class of potential-energy functions.

The clue function to be calculated first in the WKB theory is the classical momentum function. This function, for a particle of mass m and a general potential energy V, would read $p=\sqrt{2m(E-V)}$. In our case, we have got the function

$$\tilde{p}_E(\xi)=\sqrt{2\mu}\,\sqrt{E+\frac{E_{\rm g}}{2}\;-\;\frac{E_{\rm g}}{2}\sqrt{1\;+\;\frac{2\mu K}{mE_{\rm g}}\,\xi^2}}\,. \tag{6}$$

For each value $E>0$, we define the interval of the 'classical attainability', $\mathcal{I}_E\;\equiv\;(-\,b_E,b_E)$. Here $b_E>0$ has to be determined as the value of ξ equal to the positive root of the equation $\tilde{p}_E(\xi)=0$. A short calculation leads to the expression

$$b_E=\sqrt{\frac{2mE(E+E_{\rm g})}{\mu K E_{\rm g}}}\,.$$

In the spirit of the WKB theory, we write the stationary wave function corresponding to the energy E in the sine form

$$\tilde{\psi}_E(\xi)=\frac{C_E^{\rm L}}{\sqrt{\tilde{p}_E(\xi)}}\,\sin\left(\frac{1}{\hbar}\int_{-b_E}^{\xi}{\rm d}\xi'\tilde{p}_E(\xi')\;+\;\frac{\pi}{4}\right)=$$

$$=\frac{C_E^{\rm R}}{\sqrt{\tilde{p}_E(\xi)}}\,\sin\left(\frac{1}{\hbar}\int_{\xi}^{b_E}{\rm d}\xi'\tilde{p}_E(\xi')\;+\;\frac{\pi}{4}\right). \tag{7}$$

These two sines have to fit the same function. To achieve this, one has to require the fulfilment of the condition

$$\frac{1}{\hbar}\int_{-b_n}^{b_n}{\rm d}\xi\;\tilde{p}_n(\xi)=\left(n+\frac{1}{2}\right)\pi\,,\quad(n=0,1,2,\dots)\,, \tag{8}$$

where

$$\tilde{p}_n(\xi) \equiv \tilde{p}_{E_n}(\xi)\,, \quad b_n \equiv b_{E_n} = \sqrt{\frac{2mE_n(E_n+E_{\rm g})}{\mu K E_{\rm g}}}\,,$$

and to require also that the coefficients $C_E^{\rm L} \equiv C_n^{\rm L}$ and $C_E^{\rm R} \equiv C_n^{\rm R}$ have to be equal in their absolute value but with opposite signs if n is odd:

$$C_n^{\rm L} = (-1)^n C_n^{\rm R}\,.$$

For each chosen value of n $(= 0, 1, 2, \dots)$, equation (8), as a transcendental equation for E_n, has rightly one positive root.

For formal reasons, we define the dimensionless variable u and the dimensionless parameters $\beta > 0$, $A > 0$:

$$u = \sqrt{\frac{2\mu K}{mE_{\rm g}}}\,\xi\,, \quad \beta = \sqrt{\frac{2\mu K}{mE_{\rm g}}}\,b_E\,, \quad A = \frac{2E+E_{\rm g}}{E_{\rm g}} = \sqrt{\beta^2+1}\,.$$

We calculate the integral

$$\frac{E_{\rm g}}{2}\sqrt{\frac{m}{\mu K}}\,I = \int_0^{b_E} {\rm d}\xi \sqrt{E + \frac{E_{\rm g}}{2} - \frac{E_{\rm g}}{2}\sqrt{1 + \frac{2\mu K}{mE_{\rm g}}\,\xi^2}}\,,$$

i.e.

$$I = \int_0^{\beta} {\rm d}u \sqrt{A - \sqrt{u^2+1}} = \int_0^{\beta} {\rm d}u \sqrt{\sqrt{\beta^2+1} - \sqrt{u^2+1}}\,. \tag{9}$$

When making use of the variable $v = \sqrt{u^2+1}$, we transform integral (9) in the form

$$I = \int_1^A {\rm d}v \sqrt{A-v}\,\frac{v}{\sqrt{v^2-1}} = \int_1^A {\rm d}v \sqrt{A-v}\,\frac{{\rm d}\sqrt{v^2-1}}{{\rm d}v}\,.$$

When using the integration by parts, we obtain the result

$$I = \frac{1}{2}\int_1^A {\rm d}v \sqrt{\frac{v^2-1}{A-v}} = \frac{1}{2}\int_1^A {\rm d}v \sqrt{\frac{(v-1)(v+1)}{A-v}}\,.$$

In Ryzhik's and Gradshtein's book of tables [11], one finds the formula

$$\int_B^A {\rm d}v \sqrt{\frac{(v-B)(v-C)}{A-v}} = \frac{2}{3}\sqrt{A-C}\,\left[(2A-B-C)\,\mathbf{E}(\Gamma^2) - (B-C)\,\mathbf{K}(\Gamma^2)\right],$$

$$0 < \Gamma^2 = \frac{A-B}{A-C} < 1\,. \tag{10}$$

(See the expression No. 22 in Section 3.141 of [11].) This integral formula is valid with any three real parameters A, B and C provided that $A > B > C$. The symbols $\mathbf{K}(\Gamma^2)$ and $\mathbf{E}(\Gamma^2)$ signify the complete elliptic integrals of the first and of the second kind, respectively:

$$\mathbf{K}(\Gamma^2) = \int_0^{\pi/2} \frac{\mathrm{d}\varphi}{\sqrt{1-\Gamma^2\sin^2\varphi}}\,, \quad \mathbf{E}(\Gamma^2) = \int_0^{\pi/2} \mathrm{d}\varphi\,\sqrt{1-\Gamma^2\sin^2\varphi}\,.$$

Since $B = -C = 1$ in integral (10), we can rewrite equation (8) in the form

$$\frac{2E_\mathrm{g}}{3\pi}\,\sqrt{2(A+1)}\,[A\,\mathbf{E}(\Gamma^2)\;-\;\mathbf{K}(\Gamma^2)] = \hbar\omega_0\left(n+\frac{1}{2}\right).$$

Here we have introduced the frequency parameter

$$\omega_0 = \sqrt{\frac{K}{m}}$$

characterizing the oscillator under consideration. Using the explicit expressions

$$A \;\equiv\; A_n = \frac{2E_n+E_\mathrm{g}}{E_\mathrm{g}}\,, \quad \Gamma \;\equiv\; \Gamma_n = \sqrt{\frac{A_n-1}{A_n+1}} = \sqrt{\frac{E_n}{E_n+E_\mathrm{g}}}\,,$$

we obtain the final form of the equation for E_n:

$$\frac{4}{3\pi}\,\sqrt{E_\mathrm{g}(E_n+E_\mathrm{g})}\left[\frac{2E_n+E_\mathrm{g}}{E_\mathrm{g}}\,\mathbf{E}\left(\frac{E_n}{E_n+E_\mathrm{g}}\right)\;-\;\mathbf{K}\left(\frac{E_n}{E_n+E_\mathrm{g}}\right)\right] = \\ = \hbar\omega_0\left(n+\frac{1}{2}\right). \quad (11)$$

The complete elliptic integrals can be expressed as the hypergeometric series [11, 12]:

$$\mathbf{K}(\Gamma^2) = \frac{\pi}{2}\,F\left(\frac{1}{2},\frac{1}{2};1;\Gamma^2\right) = \\ = \frac{\pi}{2}\left[1\;+\;\left(\frac{1}{2}\right)^2\Gamma^2\;+\;\left(\frac{1.3}{2.4}\right)^2\Gamma^4\;+\;\left(\frac{1.3.5}{2.4.6}\right)^2\Gamma^6\;+\;\ldots\right],$$

$$\mathbf{E}(\Gamma^2) = \frac{\pi}{2}\,F\left(-\;\frac{1}{2},\frac{1}{2};1;\Gamma^2\right) = \\ = \frac{\pi}{2}\left[1\;-\;\left(\frac{1}{2}\right)^2\frac{\Gamma^2}{1}\;-\;\left(\frac{1.3}{2.4}\right)^2\frac{\Gamma^4}{3}\;-\;\left(\frac{1.3.5}{2.4.6}\right)^2\frac{\Gamma^6}{5}\;-\;\ldots\right].$$

Once we have got the solution $E_n > 0$ of equation (11), we can calculate the eigen-function $\psi_n(z)$ in the coordinate representation as the Fourier integral

$$\psi_n(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \mathrm{d}k_z \, \exp(\mathrm{i}k_z z)\phi_n(k_z) = \\ = \frac{1}{\sqrt{2\pi}} \frac{K}{E_\mathrm{g}} \int_{-\infty}^{\infty} \mathrm{d}\xi \, \exp\left(\mathrm{i}\frac{Kz}{E_\mathrm{g}}\,\xi\right)\tilde{\psi}_n(\xi)\,. \quad (12)$$

Since the function $\tilde{\psi}_n(\xi)$ itself has been expressed (by formula (7)) as an integral, expression (12) is a double integral. Nevertheless, utilizing the integration by parts, we can transform integral (12) into a single integral. Regrettably, the function $\tilde{p}(\xi)$ defined by formula (6) is fairly complicated, so we do not count on the possibility to calculate integral (12) exactly without applying a numerical method. Problems linked with the numerical calculation are merely mathematical, so we give up discussing them here. We point out only that if the value of E_n is sufficiently high, then, in order to manage effectively the calculation of integral (12), we may take advantage of the theory of asymptotic methods (cf. e.g. [13]). (In particular, we have in mind the stationary-point method.)

3 Discussion of the spectrum of the eigen-energies

Using $\hbar\omega_0$ as the energy unit, we define the dimensionless energies

$$\mathcal{E}_n = \frac{E_n}{\hbar\omega_0} \quad (13)$$

and the 'nonparabolicity parameter'

$$\alpha = \frac{\hbar\omega_0}{E_\mathrm{g}}\,. \quad (14)$$

Then (11) becomes a one-parameter equation

$$F_\alpha(\mathcal{E}_n(\alpha)) = n + \frac{1}{2}\,. \quad (15)$$

Here, in conformity with equation (11), we have defined the function

$$F_\alpha(\mathcal{E}) = \frac{4}{3\pi}\,\frac{\sqrt{1+\alpha\mathcal{E}}}{\alpha}\left[[1+2\alpha\mathcal{E}]\,\mathbf{E}\left(\frac{\alpha\mathcal{E}}{1+\alpha\mathcal{E}}\right) - \mathbf{K}\left(\frac{\alpha\mathcal{E}}{1+\alpha\mathcal{E}}\right)\right]. \quad (16)$$

When $\alpha \to +0$, the Kane function defined by expression (2) is reduced to the quadratic function,

$$\lim_{\alpha\,\to\,+0} E_\mathrm{Kane}(\mathbf{k}) = \frac{\hbar^2 k^2}{2m}\,, \quad (17)$$

and

$$F_0(\mathcal{E}) = \mathcal{E}\,. \quad (18)$$

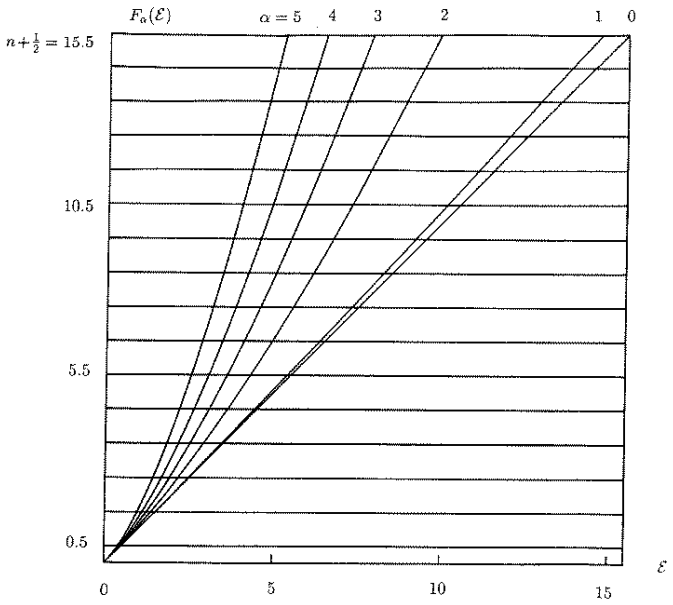

Fig. 1. Plot of the functions $F_\alpha(\mathcal{E})$ for six values of the nonparabolicity parameter α. The curves, from the right to the left, correspond to $\alpha = 0$ (the straight line) and $\alpha = 1, \ldots, 5$. The horizontal lines correspond to $n + \frac{1}{2}$ ($n = 0, \ldots, 15$).

In equation (15), we have emphasized explicitly that the energies $\mathcal{E}_n$ depend on the value of α. Within the framework of the WKB theory, equation (15) is exact and, therefore, equally usable with all positive values of α. For each quantum number n, we can easily calculate $\mathcal{E}_n(\alpha)$ in a numerical way and the algorithm of this calculation is simple. In Fig. 1, we have plotted graphs of several functions $F_\alpha(\mathcal{E})$. If $\alpha = \text{const}$, $F_\alpha(\mathcal{E})$ is an increasing function of the variable $\mathcal{E}$. The value $\mathcal{E}_n(\alpha)$ is determined as the horizontal coordinate of the intersection point of the function $F_\alpha(\mathcal{E})$ with the horizontal straight line defined by the vertical coordinate equal to $n + \frac{1}{2}$.

If the value of α is sufficiently small, we can solve equation (15) in an analytical manner. We may regard $\alpha > 0$ as a parameter of a perturbation theory. We write $E_n(\alpha)$ as a series:

$$E_n(\alpha) = \hbar\omega_0 \mathcal{E}_n(\alpha) = \hbar\omega_0 [\mathcal{E}_n^{(0)} + \mathcal{E}_n^{(1)}\alpha + \mathcal{E}_n^{(2)}\alpha^2 + \ldots]$$

A straightforward calculation—see Appendix—gives us the value

$$E_n(0) = \hbar\omega_0 \mathcal{E}_n^{(0)} = \hbar\omega_0 \left(n + \frac{1}{2} \right) .$$

This is the well-known result valid for a linear harmonic oscillator.

In Appendix, we calculate also the coefficient $\mathcal{E}_n^{(1)}$. According to our calculations, the first-

	$\alpha = 0$	$\alpha = 0.1$	$\alpha = 0.2$	$\alpha = 0.5$	$\alpha = 1$	$\alpha = 2$
n	$\mathcal{E}_n(0)$	$\mathcal{E}_n(0.1)$	$\mathcal{E}_n(0.2)$	$\mathcal{E}_n(0.5)$	$\mathcal{E}_n(1)$	$\mathcal{E}_n(2)$
0	0.5	0.49105	0.48285	0.46177	0.43460	0.39672
1	1.5	1.42589	1.36700	1.24098	1.11130	0.96438
2	2.5	2.30885	2.17300	1.91280	1.67308	1.42297
3	3.5	3.14955	2.92234	2.51905	2.17205	1.82643
4	4.5	3.95491	3.62799	3.07945	2.62929	2.19434
5	5.5	4.73007	4.29850	3.60524	3.05595	2.53665
6	6.5	5.47902	4.93986	4.10361	3.45885	2.85926
7	7.5	6.20492	5.55650	4.57946	3.84250	3.16603
8	8.5	6.91031	6.15180	5.03637	4.21012	3.45969
9	9.5	7.59729	6.72840	5.47701	4.56408	3.74222
10	10.5	8.26761	7.28842	5.90347	4.90621	4.01512
11	11.5	8.92275	7.83361	6.31740	5.23794	4.27960
12	12.5	9.56398	8.36539	6.72015	5.56043	4.53660
13	13.5	10.1924	8.88499	7.11284	5.87463	4.78690
14	14.5	10.8089	9.39344	7.49640	6.18132	5.03116
15	15.5	11.4144	9.89164	7.97160	6.48118	5.26990

Tab. 1. Some WKB exact values of $\mathcal{E}_n(\alpha)$ calculated from equation (15)

order perturbation theory (with respect to α) leads to the formula

$$E_n(\alpha) = \hbar\omega_0\left(n+\frac{1}{2}\right)\left[1\ -\ \frac{3\alpha}{8}\left(n+\frac{1}{2}\right)\right]\ +\ \mathcal{O}(\alpha^2)\,. \tag{19}$$

In Tab. 1, we present some values of $\mathcal{E}_n(\alpha)$. Since these values have been calculated from equation (15), we consider them as 'WKB exact'. The purpose of Tab. 2 is to illustrate the accuracy of the 'WKB linear approximation' which means that the values of $\mathcal{E}_n(\alpha)$ are calculated according to formula (19) with neglecting all terms $\mathcal{O}(\alpha^2)$. For a given value of α, the 'WKB linear approximation' becomes worse and worse as the index n grows. The 'WKB linear' value of $\mathcal{E}_n(\alpha)$ is always lower than the corresponding 'WKB exact' value. With $\alpha = 0.1$, the discrepancy between these values does not exceed 10 per cent for $0 \leq n \leq 5$, whilst for $\alpha = 0.5$, the discrepancy does already exceed 10 per cent if $n \geq 1$. If $\alpha > 1$, the accuracy of the 'WKB linear approximation' is practically not tolerable. (If $\alpha = 1$, then even for the lowest eigen-energy, when $n = 0$, the discrepancy between the corresponding 'WKB linear' and 'WKB exact' values of $\mathcal{E}_0(1)$ is about 6.52 per cent. If $\alpha = 2$, this dicrepancy would be about 21.23 per cent!)

An improvement could be, of course, realised if the second-order perturbation theory (with respect to α) were taken into account. We could generalize formula (19) by extending the calculations of Appendix. Nonetheless, the 'WKB exact' calculation employing equation (15) is so simple that, we believe, we need not further to work up the perturbation theory in more detail.

If the value of n is fixed, the function $E_n(\alpha)$ decreases asymptotically to zero if α tends to infinity. To prove this statement, let us take $\mathcal{E} = \mathrm{const}$ and analyze the asymptotic behaviour of

$\alpha = 0.1$			
n	$\mathcal{E}_n^{\rm exact}(\alpha)$	$\mathcal{E}_n^{\rm linear}(\alpha)$	$\delta\mathcal{E}_n(\alpha)$
0	0.49105	0.490625	0.09
1	1.42589	1.415625	0.72
2	2.30885	2.265625	1.87
3	3.14955	3.040625	3.46
4	3.95491	3.740625	5.42
5	4.73007	4.365625	7.70
6	5.47902	4.915625	10.28

$\alpha = 0.2$			
n	$\mathcal{E}_n^{\rm exact}(\alpha)$	$\mathcal{E}_n^{\rm linear}(\alpha)$	$\delta\mathcal{E}_n(\alpha)$
0	0.48285	0.48125	0.33
1	1.36700	1.33125	2.62
2	2.17300	2.03125	6.52
3	2.92234	2.58125	11.67

$\alpha = 0.5$			
n	$\mathcal{E}_n^{\rm exact}(\alpha)$	$\mathcal{E}_n^{\rm linear}(\alpha)$	$\delta\mathcal{E}_n(\alpha)$
0	0.46177	0.453125	1.87
1	1.24098	1.078125	13.12

$\alpha = 1$			
n	$\mathcal{E}_n^{\rm exact}(\alpha)$	$\mathcal{E}_n^{\rm linear}(\alpha)$	$\delta\mathcal{E}_n(\alpha)$
0	0.43460	0.40625	6.52
1	1.11130	0.65625	40.95

$\alpha = 2$			
n	$\mathcal{E}_n^{\rm exact}(\alpha)$	$\mathcal{E}_n^{\rm linear}(\alpha)$	$\delta\mathcal{E}_n(\alpha)$
0	0.39672	0.3125	21.23

Tab. 2. Comparison of 'WKB exact' with 'WKB linear' values of $\mathcal{E}_n(\alpha)$. In this Table, $\delta\mathcal{E}_n(\alpha) = 100\times[\mathcal{E}_n^{\rm exact}(\alpha)-\mathcal{E}_n^{\rm linear}(\alpha)]/\mathcal{E}_n^{\rm exact}(\alpha)$ means the percentage in which $\mathcal{E}_n^{\rm linear}(\alpha)$ differs from $\mathcal{E}_n^{\rm exact}(\alpha)$. Tab. 2 is composed of five partial tables. With any fixed value of α, the sequence $\delta\mathcal{E}_0(\alpha)$, $\delta\mathcal{E}_1(\alpha)$, $\delta\mathcal{E}_2(\alpha)$, ... increases. The last row in each partial table corresponds to the first value of the oscillator quantum number, $n = \tilde{n}(\alpha)$, for which $\delta\mathcal{E}_n(\alpha)$ exceeds ten per cent. The values of $\mathcal{E}_n^{\rm exact}(\alpha)$, $\mathcal{E}_n^{\rm linear}(\alpha)$ and $\delta\mathcal{E}_n(\alpha)$ for $n > \tilde{n}(\alpha)$ have not been included in these tables.

the function $F_\alpha(\mathcal{E})$ (cf. expression (16)) for $\alpha \to \infty$. The complete elliptic integral $\mathbf{K}(\Gamma^2)$ diverges logarithmically if $\Gamma \to 1$ from the left [11]. Indeed, if $\alpha \to \infty$,

$$\mathbf{K}\left(\frac{\alpha\mathcal{E}}{1+\alpha\mathcal{E}}\right) = \mathbf{K}\left(1 - \frac{1}{1+\alpha\mathcal{E}}\right) = \ln\left(4\sqrt{1+\alpha\mathcal{E}}\,\right)\left[1 + \mathcal{O}\left(\frac{1}{\alpha}\right)\right].$$

On the other hand,

$$\mathbf{E}\left(\frac{\alpha\mathcal{E}}{1+\alpha\mathcal{E}}\right) = \mathbf{E}\left(1 - \frac{1}{1+\alpha\mathcal{E}}\right) = 1 + \frac{1}{2}\,\ln\left(4\sqrt{1+\alpha\mathcal{E}}\,\right)\mathcal{O}\left(\frac{1}{\alpha}\right).$$

Thus, the leading term in the large brackets $[\dots]$ in expression (16) is $2\alpha\mathcal{E}$ and we may write the asymptotic expression for $F_\alpha(\mathcal{E})$:

$$F_\alpha(\mathcal{E}) \approx \frac{8}{3\pi}\,\alpha^{1/2}\mathcal{E}^{3/2}\,.$$

(Here we have neglected unity against $\alpha\mathcal{E}$.) Hence, equation (15) gives us the asymptotic solution

$$\mathcal{E}_n(\alpha) \approx \left(\frac{3\pi}{8}\right)^{2/3}\left(n+\frac{1}{2}\right)^{2/3}\frac{1}{\alpha^{1/3}}$$

for $\alpha \to \infty$.

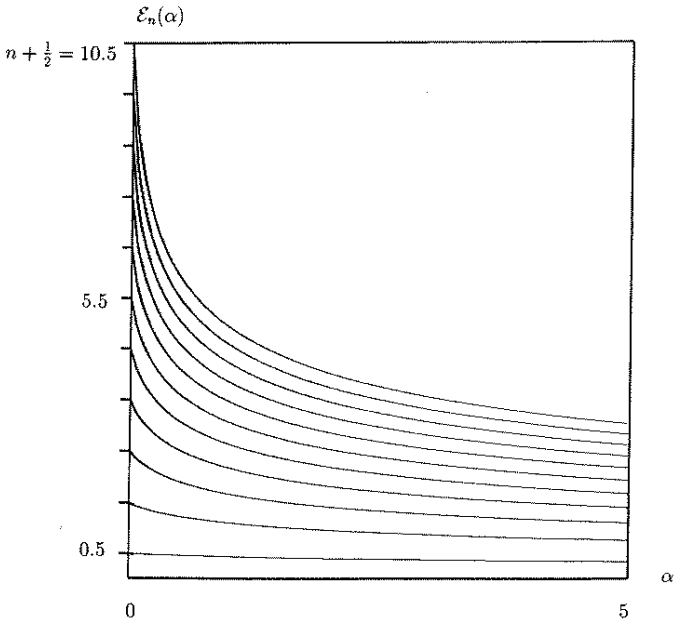

Fig. 2. Plot of the functions $\mathcal{E}_n(\alpha)$ for eleven values of the quantum number n. From below upwards, $n = 0, 1, \ldots, 10$. The scale of α is linear. The curves start, at $\alpha = 0$, from $\mathcal{E}_n(0) = n + \frac{1}{2}$.

In Fig. 2, we have shown the functions $\mathcal{E}_n(\alpha)$ for the lowest eleven values of n. Clearly, the function $E_n(\alpha)$ decreases most steeply at $\alpha \to +0$ and if we compare the functions $E_n(\alpha)$ with different indices n, we observe that the steepness of the decrease of these functions at $\alpha \to +0$ grows with n. This affirmation does also follow from formula (19) which yields us the derivative

$$\left.\frac{\partial \mathcal{E}_n(\alpha)}{\partial \alpha}\right|_{\alpha=+0} = -\frac{3}{8}\left(n+\frac{1}{2}\right)^2.$$

4 Concluding remarks

In this paper, we have solved the one-dimensional Schrödinger-Wannier equation

$$E\left(\mathrm{i}\frac{\partial}{\partial z}\right)\psi_n(z) + \frac{1}{2}Kz^2\psi_n(z) = E_n\psi_n(z)$$

with $E(k_z)$ chosen in the form of the Kane function $E_{\mathrm{Kane}}(k_z)$. (Cf. expression (2) with $k_x = k_y = 0$.) Obviously, the method which we have employed in this paper, based on the quasi-classical approximation (WKB approximation), is equally applicable with many other adequate

functions $E(k_z)$. Generally, in correspondence to the choice of $E(k_z)$, we may speak, when discussing quantum thin films modelled by a quadratic confining potential, not only of the Kane oscillator but also of other oscillators that are different from the common quantum-mechanical harmonic oscillator.

Here it should be pointed out that realistic functions $E(k_z)$, as a rule, resemble the quadratic function $\hbar^2 k_z^2/(2m)$ in a wide enough interval of k_z around the point $k_{0z} = 0$. This is a favourable aspect for our theory since, as it was well known from the very discovery of the quantum mechanics, the WKB approximation gives *exact* results for *all* eigen-energies of the harmonic oscillator, i.e. also for low-lying energies E_n. On the other hand, *in general*, if the potential energy is not quadratic, the WKB approximation holds as a *high-energy approximation*. In our theory, we have used the k_z-representation. Then the dispersion function $E(k_z)$ plays the role of a 'potential energy' which behaves quadratically in a relatively wide interval around the central point $k_{0z} = 0$, but non-quadratically at high values of $|k_z|$. Therefore, there is a good reason to believe that for a broad class of dispersion functions $E(k_z)$, the WKB approximation may provide, at least in the case of the quadratic potential energy $V(z) = \frac{1}{2}Kz^2$ (which, in the k_z-representation becomes the 'kinetic-energy' operator $-\frac{1}{2}K\partial^2/\partial k_z^2$), quite good values both for low-lying and for high-lying eigen-energies E_n. For energies in between, the WKB approximation may still be deemed reasonable as a natural interpolation between two regions where the suitability of this approximation was well established.

Our second remark concerns the dependence of the oscillator eigen-energies on the nonparabolicity parameter $\alpha \sim 1/E_{\rm G}$. We can clarify why $E_{\rm g}(\alpha)$ are decreasing functions of α as follows. The Kane electron is a quasi-particle whose effective mass grows with energy. Indeed, what we have denoted as m is the effective mass at $E = 0$. For $E > 0$, the effective mass $m_{\rm Kane}(E)$ of the Kane electron is defined by the formula [9]

$$\frac{1}{m_{\rm Kane}(E)} = \frac{1}{\hbar^2}\,\frac{\partial^2 E_{\rm Kane}(k_z)}{\partial k_z^2}\,,$$

which gives the function

$$m_{\rm Kane}(E) = m\left(1 + \frac{2E}{E_{\rm g}}\right)^3,$$

or, if we use the denotation $\tilde{m}_{\rm Kane}(\mathcal{E}) \equiv m_{\rm Kane}(E)$, the function

$$\tilde{m}(\mathcal{E}) = m\,(1 + 2\alpha\mathcal{E})^3\,.$$

Thus, the Kane electron, when oscillating in a potential well defined by the function $V(z)$, keeps actually moving like a heavier quasi-particle than the 'free electron' of mass m: the heavier, the higher the value of the energy E_n is and the higher the value of the nonparabolicity parameter is. Only if $\alpha = 0$, the electron is 'light', with the effective mass m which is energy-independent.

Our conclusion that the values of the eigen-energies E_n decrease if $1/E_{\rm g}$ increases (i.e. if $E_{\rm g}$ decreases) is valid quite generally, whichever the shape of the potential-well function $V(z)$ is. To exemplify this conclusion, let us now discuss the 1D Sommerfeld model. In this case, the eigen-functions of the Kane electron are $\psi_n(z) \sim \sin(\pi n z/a)$, where $a > 0$ is the width of the well and $n = 1, 2, \ldots$ Correspondingly, the Sommerfeld-Kane eigen-energies are

$$E_n^{\rm SK}\left(\frac{1}{E_{\rm g}}\right) = \frac{E_{\rm g}}{2}\left[\left(1 + \frac{2\pi^2\hbar^2 n^2}{ma^2 E_{\rm g}}\right)^{1/2} - 1\right]$$

and, clearly,

$$E_n^{\mathrm{SK}}\left(\frac{1}{E_{\mathrm{g}}}\right) < E_n^{\mathrm{SK}}(0) = \frac{\pi^2\hbar^2 n^2}{2ma^2}$$

for $0 < E_{\mathrm{g}} < \infty$.

Finally, let us point out that although we have applied the WKB approach to the 1D Kane oscillator, there would be no hindrance to apply it to 2D and 3D Kane (and other) oscillators.

Appendix

We write

$$\mathcal{E}_n(\alpha) = \mathcal{E}_n^{(0)} + \mathcal{E}_n^{(1)}\alpha + \mathcal{E}_n^{(2)}\alpha^2 + \mathcal{O}(\alpha^3)\,.$$

If α is small, we may approximate relevant expressions in the l.h.s. of equation (17) by polynomials. As the prefactor in function (16) involves α in the denominator, then, to obtain the coefficients $\mathcal{E}_n^{(0)}$ and $\mathcal{E}_n^{(1)}$, we may confine ourselves to considering the remaining expressions in formula (16) as the second-order polynomials. Thus we write the following expressions:

$$\sqrt{1+\alpha\mathcal{E}_n(\alpha)} = 1 \,+\, \frac{\mathcal{E}_n^{(0)}}{2}\,\alpha \,+\, \frac{4\mathcal{E}_n^{(1)} - [\mathcal{E}_n^{(0)}]^2}{8}\,\alpha^2 \,+\, \mathcal{O}(\alpha^3)\,,$$

$$1 + 2\alpha\mathcal{E}_n(\alpha) = 1 + 2\mathcal{E}_n^{(0)}\alpha + 2\mathcal{E}_n^{(1)}\alpha^2 + \mathcal{O}(\alpha^3)\,,$$

$$\frac{\alpha\mathcal{E}_n(\alpha)}{1+\alpha\mathcal{E}_n(\alpha)} = \mathcal{E}_n^{(0)}\alpha + (\mathcal{E}_n^{(1)} - [\mathcal{E}_n^{(0)}]^2)\,\alpha^2 + \mathcal{O}(\alpha^3)\,,$$

$$\mathbf{K}\left(\frac{\alpha\mathcal{E}_n(\alpha)}{1+\alpha\mathcal{E}_n(\alpha)}\right) = \frac{\pi}{2}\left[1 \,+\, \frac{\alpha\mathcal{E}_n(\alpha)}{4[1+\alpha\mathcal{E}_n(\alpha)]} \,+\, \frac{9}{64}\left(\frac{\alpha\mathcal{E}_n(\alpha)}{1+\alpha\mathcal{E}_n(\alpha)}\right)^2 \,+\, \mathcal{O}(\alpha^3)\right] =$$
$$= \frac{\pi}{2}\left[1 \,+\, \frac{\mathcal{E}_n^{(0)}}{4}\,\alpha \,+\, \frac{16\mathcal{E}_n^{(1)} - 7[\mathcal{E}_n^{(0)}]^2}{64}\,\alpha^2 \,+\, \mathcal{O}(\alpha^3)\right],$$

$$\mathbf{E}\left(\frac{\alpha\mathcal{E}_n(\alpha)}{1+\alpha\mathcal{E}_n(\alpha)}\right) = \frac{\pi}{2}\left[1 \,-\, \frac{\alpha\mathcal{E}_n(\alpha)}{4[1+\alpha\mathcal{E}_n(\alpha)]} \,-\, \frac{3}{64}\left(\frac{\alpha\mathcal{E}_n(\alpha)}{1+\alpha\mathcal{E}_n(\alpha)}\right)^2 \,+\, \mathcal{O}(\alpha^3)\right] =$$
$$= \frac{\pi}{2}\left[1 \,-\, \frac{\mathcal{E}_n^{(0)}\alpha}{4} \,-\, \frac{16\mathcal{E}_n^{(1)} - 13[\mathcal{E}_n^{(0)}]^2}{64}\,\alpha^2 \,+\, \mathcal{O}(\alpha^3)\right],$$

Equation (15) has the structure

$$\frac{4}{3\pi}\,\frac{\sqrt{1+\alpha\mathcal{E}_n(\alpha)}}{\alpha}\left[\,\ldots\,\right] = \frac{4}{3\pi\alpha}\left(1 + \frac{\mathcal{E}_n^{(0)}}{2}\,\alpha + \frac{4\mathcal{E}_n^{(1)} - [\mathcal{E}_n^{(0)}]^2}{8}\,\alpha^2 + \mathcal{O}(\alpha^3)\right)\left[\,\ldots\,\right] =$$
$$= n + \frac{1}{2}\,,$$

where

$$\Big[\,\ldots\,\Big] = [1+2\alpha\mathcal{E}_n(\alpha)]\,\mathbf{E}\Big(\frac{\alpha\mathcal{E}_n(\alpha)}{1+\alpha\mathcal{E}_n(\alpha)}\Big)\;-\;\mathbf{K}\Big(\frac{\alpha\mathcal{E}_n(\alpha)}{1+\alpha\mathcal{E}_n(\alpha)}\Big) =$$

$$= \frac{3\pi\alpha}{4}\left(\mathcal{E}_n^{(0)}\;+\;\frac{8\mathcal{E}_n^{(1)}-[\mathcal{E}_n^{(0)}]^2}{8}\,\alpha\right)\;+\;\mathcal{O}(\alpha^3)\,.$$

Hence,

$$\frac{4}{3\pi\alpha}\,\sqrt{1+\alpha\mathcal{E}_n(\alpha)}\Big[\,\ldots\,\Big] = \left(1\;+\;\frac{\mathcal{E}_n^{(0)}}{2}\,\alpha\right)\left(\mathcal{E}_n^{(0)}\;+\;\frac{8\mathcal{E}_n^{(1)}-[\mathcal{E}_n^{(0)}]^2}{8}\,\alpha\right)\;+\;\mathcal{O}(\alpha^2) =$$

$$= \mathcal{E}_n^{(0)}\;+\;\left(\mathcal{E}_n^{(1)}\;+\;\frac{3}{8}\,[\mathcal{E}_n^{(0)}]^2\right)\alpha\;+\;\mathcal{O}(\alpha^2) = n+\frac{1}{2}\,.$$

In this way, we have obtained the values:

$$\mathcal{E}_n^{(0)} = n+\frac{1}{2}$$

and

$$\mathcal{E}_n^{(1)} = -\,\frac{3}{8}\,[\mathcal{E}_n^{(0)}]^2\,.$$

Therefore,

$$\mathcal{E}_n(\alpha) = \left(n+\frac{1}{2}\right)\left[1\;-\;\frac{3\alpha}{8}\left(n+\frac{1}{2}\right)\right]\;+\;\mathcal{O}(\alpha^2)\,.$$

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