

SEPARATION OF THE SCHRÖDINGER EQUATION IN THIN FILMS

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The restriction of the thickness dimension of thin films is directly used in an analysis of the general problem of electrons in thin films, resulting in a Born-Oppenheimer-like approximate separation of the problem.

The study of electrons in thin films is a very interesting subject and considerable theoretical work [1-6] has been done in it in recent times. The analyses, however, seem either to deal with specific simple models [2, 4, 5] or to assume the effective mass approximation [1, 6]. One thus encounters in the literature, harmonic oscillator models, or free electrons of modified mass contained in a box of impenetrable walls. An analysis of the general model-independent problem of an electron in a thin film does not seem to have been carried out. In this letter we write the general Hamiltonian and show that the fact that we have a thin film and not a bulk sample, allows us to carry out a certain separation of the problem, patterned after the Born-Oppenheimer approximation [7, 8] in solids.

The Schrödinger equation, for each of the non-interacting electrons,

$$-\frac{\hbar^2}{2m} \left\{ \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right\} + V(x, y, z) \psi = E \psi \quad (1)$$

is trivially separable if the interaction $V(x, y, z)$ satisfies

$$V(x, y, z) = V_1(x, y) + V_2(z) \quad (2)$$

While the models in the literature do satisfy (2), it is a highly stringent condition and there is no reason to believe that real films satisfy it even approximately. Our analysis here begins by noticing, either from the detailed analysis of a simple model (for instance free electrons in a box), or from the uncertainty principle, that for the low-lying states (see fig. 1) the value of p_z (momentum component in the z -direction) is much higher than the value of p_x or p_y . For these states therefore, the kinetic energy due to the z -motion (or $\partial^2 \psi / \partial z^2$) is much larger than that due to the xy -motion (or $\partial^2 \psi / \partial x^2 + \partial^2 \psi / \partial y^2$). This important result, which is a consequence of the smallness of the ratio d/L of the film thickness to a normalizing length in the x or y direction, is reminiscent of the Born-Oppenheimer approximation [7, 8] where a separation of the problem into an electron part and an ion part is made possible by the smallness of the mass ratio. We therefore consider, along parallel lines,

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \phi(x, y, z)}{\partial z^2} + V(x, y, z) \phi(x, y, z) = \mathcal{E}(x, y) \phi(x, y, z) \quad (3)$$

and attempt a solution of (1) in the form

$$\psi(x, y, z) = \sum_i \eta_i(x, y) \phi_i(x, y, z) \quad (4)$$

where ϕ_i are the eigenfunctions of (3) with eigenvalues \mathcal{E}_i . We get

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \eta_j + [\mathcal{E}_j(x, y) - E] \eta_j - \left\{ \frac{\hbar^2}{2m} \sum_i \eta_i \langle \phi_j | \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) | \phi_i \rangle + \frac{\hbar^2}{m} \sum_i \langle \phi_j | \left(\frac{\partial \eta_i}{\partial x} \frac{\partial}{\partial x} + \frac{\partial \eta_i}{\partial y} \frac{\partial}{\partial y} \right) | \phi_i \rangle \right\} = 0 \quad (5)$$

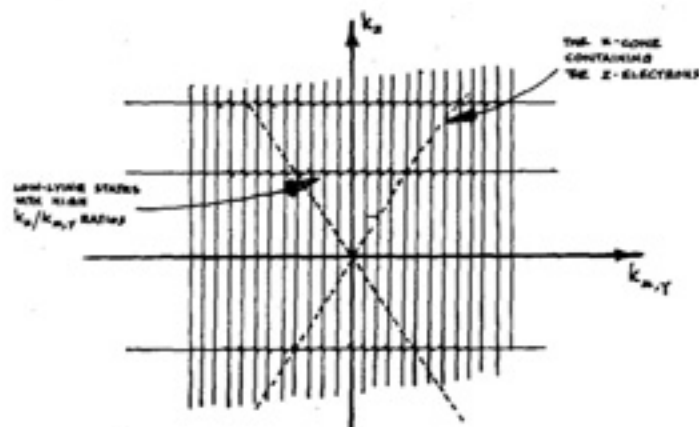
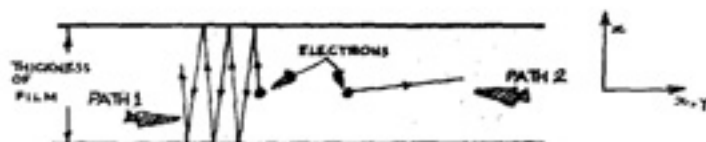
Fig. 1. Quantum levels of the film showing the z -cone.

Fig. 2. Typical electron paths in the thin film.

and if the terms in the curly brackets are in some sense negligible we have

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) \eta_j(x, y) + \mathcal{E}_j(x, y) \eta_j(x, y) = E \eta_j(x, y). \quad (6)$$

We thus have two separate problems: (3) in the z -direction and (6) in the x - y plane. When such a separation is valid one may therefore treat the x - y problem independently exactly as one might in a two-dimensional bulk sample and then append to the results in a fairly direct manner, the solution of the one-dimensional problem in the z -direction. The energies merely add and one may confidently discuss the formation of sub-bands and such other effects as are discussed in the free-electron case (e.g., ref. [1]). This separation is valid not only for the low-lying states but also for certain other states. In fact, as one goes up the energy scale, the separation scheme holds well and breaks down alternately, with the consequence that the electrons for which the separation is valid (which we term the z -electrons), occupy states, which maybe loosely asserted to lie in a cone around the k_z -axis, with an appropriate angle (see fig. 1). The interesting fact is that it is exactly these z -electrons which mainly contribute to phenomena that depend on the film-character of the sample - as is evident from fig. 2: the z -electrons travel along "paths" of type 1. (The latter statement is valid for all thermodynamic properties and for most kinetic properties except in situations involving an external longitudinal magnetic field.)

The preceding discussion thus shows that while the Hamiltonian of the electrons is not separable at all when the sample is in bulk form, the restriction on one of the dimensions, that appears in a thin film, immediately results in one's being able to choose a group of electrons for which a separation can be carried out to a good approximation. This analysis, within its range of validity, thus provides sound justification for the model-calculations [1-6] in the literature.

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