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Effective-Mass Approximation for Bloch Electrons in Finite-Range Constant Electric Fields*

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Contrary to the inability to use the effective-mass approximation (EMA) for infinite crystals, two criteria are obtained for the validity of the EMA for finite crystals. The first restricts the potential drop across the crystal to be less than the band gap, and the second restricts the "empty-lattice" energy level to be smaller than the free-electron kinetic energy.

I. INTRODUCTION

The dynamics of Bloch electrons in the presence of external fields can, under certain conditions, be made very simple by the use of the effective-mass approximation (EMA). The criteria for the validity of this approximation for the impurity case and for a crystal in a constant magnetic field were obtained by Luttinger and Kohn[1] and, for the former case, also by Zak[2] using his kq representation and deriving the next term in this approximation. The case of crossed electric and magnetic fields was treated by Zak and Zawadski.[3] Usually these criteria are given by the "gentleness" of the perturbing potential[1] and by the smoothness of the wave functions.[2-4] None of these works is concerned with the case of a finite crystal.

In the case of an applied constant electric field the EMA has been used[5] to calculate the electro-optic absorption.[6,7] The functions used for the calculation were of the Kohn-Luttinger[1] type, with solutions for the infinite range "empty crystal" in the presence of the field multiplying the Bloch functions. This approach resulted in energies in the presence of the field ranging from $-\infty$ to $+\infty$ even for the smallest electric field and so it is hard to explain the use of the EMA there. In fact, one can easily show that an infinite crystal in a constant electric field constitutes a problem which cannot be simplified by the effective-mass approximation. To see this we note that one of the conditions for the validity of the EMA is the smoothness of the effective eigenfunctions,[3,4] namely, the demand that the functions can be developed with a small number of Fourier components. [See also condition (b) in this paper and its discussion following Eq. (2.32).] Now, the Fourier transform of the Airy function $\mathrm{Ai}(x)$, which is the effective solution for the infinite crystal, is given[8] by

$$\mathrm{Ai}(x) = \tfrac{1}{2}\int_{-\infty}^{\infty} e^{ikx} e^{ik^3/3}\, dk,$$

the components being of order 1 in absolute value for the whole k axis. Thus the smoothness is not fulfilled in the infinite case and the EMA is not valid.

In this paper we try to investigate conditions under which the problem of an electron in a *finite* crystal in an external field can be approximated by the EMA. As the finite problem has some unique properties hitherto untreated, we rederive the approximation for this case. We follow the Luttinger-Kohn method of investigating the validity of the EMA, and we stress the different features and also some assumptions implied in Ref. 1 but not elaborated upon. We restrict ourselves to the one-dimensional case. The three-dimensional one is a readily obtained extension of the present treatment. We shall see that several steps of the proof are easier in the finite-crystal case.

In the specific case treated in this paper, namely, the constant electric field, the potential is "gentle" enough, being a first-degree polynomial in x [see also Eq. (2.21) ff] and we get two conditions [strictly speaking sufficient conditions but not necessary ones (like the criteria obtained previously[1-4])] for the validity of the EMA here. The first (C 1)

follows from the demand that the Fourier components of the potential be smaller than a typical interband separation, and the second (C 2) follows from the wanted smoothness for the effective wave function.

II. EMA

We consider electrons inside a finite one-dimensional crystal governed by the time-independent Schrödinger equation

$$[p^2/2M + V(x) + U(x)]\Psi(x) = \epsilon\Psi(x) ,$$

$$0 \leq x \leq Na = L \quad (2.1)$$

where $V(x) = V(x+a)$ is the crystal periodic potential with a period a.

$U(x)$ is the additional potential which in our case is eEx. For boundary conditions we shall use the appropriate[9] periodic ones

$$\Psi(0) = \Psi(L), \quad \frac{\partial\Psi}{\partial x}(0) = \frac{\partial\Psi}{\partial x}(L). \quad (2.2)$$

The solutions of (2.1) and (2.2) with $U = 0$ are the (assumed known) Bloch functions

$$\varphi_{n,m}(x) = e^{i(2\pi/L)mx} u_{nm}(x),$$

$$m = 0, 1, \ldots, N-1 \quad (2.3)$$

and eigenvalues $\epsilon_n(m)$. The $\varphi_{n,m}$ constitute a complete orthonormal set,

$$\langle \varphi_{n'm'} \mid \varphi_{nm} \rangle = \delta_{nn'}\,\delta_{mm'} . \quad (2.4)$$

If we carry out the integration by dividing the crystal into unit cells and summing the integrals over these, we get

$$\langle \varphi_{n'm'} \mid \varphi_{nm} \rangle = N\delta_{mm'} \int_0^a u^*_{n'm} u_{nm}\, dx ,$$

where we made use of the identity

$$\sum_{p=0}^{N-1} e^{i(2\pi/L)(m-m')la} = N\delta_{mm'} . \quad (2.5)$$

In what follows we shall use the relation (for $m = m'$)

$$\int_0^a u_{n'm}(x) u_{nm}(x)\, dx = N^{-1}\delta_{nn'} . \quad (2.6)$$

Now we prove that the following set: $\chi_{nm} = e^{i2\pi mx/L} \times U_{n,0}(x)$ is a complete set if $\{\varphi\}$ is. This can be proved relatively more easily for the finite case than for the infinite one.[1] First we show that $\{u_{n,0}(x)\}$ is a complete set for periodic functions. Every function $f(x)$ can be developed in the φ-s:

$$f(x) = \sum_n \sum_{m=0}^{N-1} g_{nm}\varphi_{nm}(x) , \quad (2.7)$$

where

$$g_{nm} = \int_0^L f(x)\,\varphi^*_{nm}(x)\, dx$$

$$= \int_0^L f(x) e^{i2\pi mx/L} u^*_{nm}(x)\, dx . \quad (2.8)$$

Now, if $f(x+a) = f(x)$ we can develop $f(x)u^*_{nm}(x)$ in a Fourier series:

$$f(x)\, u^*_{nm}(x) = \sum_l B^{nm}_l e^{i2\pi lx/a} , \quad (2.9)$$

where

$$B^{nm}_l = \frac{1}{a}\int_0^a f(x)\, u^*_{nm}(x) e^{-i2\pi lx/L}\, dx . \quad (2.10)$$

In this case,

$$g_{nm} = \sum_l B^{nm}_l \int_0^L e^{i2\pi x(lN-m)/L}\, dx = LB^{n,0}_0\,\delta_{m,0} \quad (2.11)$$

so that, from (2.7) and (2.10),

$$f(x) = \sum_n g_{n,0} u_{n,0}(x)$$

$$= N\int_0^a f(x')\, dx' \sum_n u^*_{n0}(x')\, u_{n0}(x) \quad (2.12)$$

(f is periodic) and thus $\{u_{n0}(x)\}$ is a complete set for periodic functions.

Now, if $\psi(x)$ is a general function (not periodic), we have that $\{\chi_{nm}\}$ is a complete set, because from (2.7), using (2.12) for the periodic functions $u_{nm}(x)$ and the definition of $\chi_{nm}(x)$,

$$\psi(x) = \sum_{n,m} G_{nm}\chi_{nm}(x), \quad (2.13)$$

where

$$G_{nm} = \sum_l g_{ml} b^{lm}_n$$

and the $g_{m,n}$ are the coefficients in the development of ψ in Bloch functions (2.7), and the b^{lm}_n are the development coefficients of the periodic $u_{l,m}(x)$ in terms of the $\{u_{n,0}(x)\}$,

$$u_{l,m}(x) = \sum_n b^{lm}_n u_{n0}(x).$$

The orthonormality of the χ's is also easily proved:

$$\langle \chi_{nm} \mid \chi_{n'm'} \rangle = \int_0^L e^{i2\pi(m'-m)x/L} u^*_{n0} u_{n'0}\, dx . \quad (2.14)$$

The term in the integrand multiplying the exponent is periodic and so can be developed in Fourier series:

$$u^*_{n0}(x) u_{n'0}(x) = \sum_l B^{nn'}_l e^{i2\pi lx/a} , \quad (2.15)$$

where

$$B^{nn'}_l = \frac{1}{a}\int_0^a u^*_{n0}(x) u_{n'0}(x)\, e^{-i2\pi lx/a}\, dx. \quad (2.16)$$

Inserting (2.15) in (2.14), we have

$$\langle \chi_{nm} \mid \chi_{n'm'} \rangle = L \sum_l B_l^{mm'} \delta_{Nl+m-m',0} ,$$

where we used the identity

$$\int_0^L e^{i2\pi px/L} dx = L\delta_{p,0} .$$

But $m'-m$ ranges only between $-(N-1)$ and $(N-1)$. So l in the above δ function can be only 0 and we have, using (2.6),

$$\langle \chi_{nm} \mid \chi_{n'm'} \rangle = LB_0^{mm'} \delta_{mm'} = \delta_{nn'} \delta_{mm'} . \qquad (2.17)$$

In this way we have built a Luttinger-Kohn–type finite orthonormal complete set of functions for the interval $[0, L]$. Next we derive the appropriate Schrödinger equation in this representation. To this end we multiply (2.1) by $\chi^*_{nm}(x)$ and integrate from 0 to L. From the first term we get

$$-\frac{\hbar^2}{2M}\left[\chi^*_{nm}\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\chi^*_{nm}}{\partial x}\right]_0^L + \int_0^L \Psi\frac{\partial^2}{\partial x^2}\chi^*_{nm}\,dx .$$

With the "appropriate" boundary conditions [i.e., those for which the Wronskian vanishes, e.g., (2.2)], the Hamiltonian is Hermitian. Using (2.13), (2.17), and the definition of $u_{n,0}$, we get from (2.1) (assuming the order of summation and integration can be interchanged)

$$\frac{\hbar}{M}\frac{2\pi m}{L}\sum_n p_{nn'} G_{n'm} + \left[\epsilon_n(0) + \frac{\hbar^2}{2M}\left(\frac{2\pi m}{L}\right)^2 - \epsilon\right] G_{nm} + \int_0^L U(x)\Psi(x)\chi^*_{nm}(x)\,dx = 0 , \qquad (2.18)$$

where[1]

$$p_{nn'} = N\int_0^a u^*_{n0}\hat{p}\,u_{n'0}\,dx .$$

In deriving (2.18) we used the identity [for periodic functions $f(x)$]

$$\int_0^L e^{i2\pi x(m'-m)/L} f(x)\,dx = N\delta_{mm'}\int_0^a f(x)\,dx , \qquad (2.19)$$

which is equivalent to the treatment in (2.14)–(2.17). In the last term of (2.18) $U(x)$ is bounded [in our case $U(x) = eEx \le eEL$], and thus the last term can be written in the form

$$I = \sum_{n'm'} G_{n'm'}\int_0^L U(x)u_{n'0}(x)u^*_{n0}(x)\,e^{i2\pi x(m'-m)/L}\,dx .$$

Expanding $u^*_{n,0}u_{n',0}$ in Fourier series (2.15) we get

$$I = L\sum_{n'l} B_l^{mm'}\sum_{m'} G_{n'm'}\,\bar{U}(lN+m'-m) , \qquad (2.20)$$

where $\bar{U}(p) = L^{-1}\int_0^L U(x)e^{i2\pi px/L}\,dx$ is the Fourier transform of $U(x)$ in the interval. In our case $U(x) = eEx$, so

$$\bar{U}(lN+m'-m) = \frac{lEL}{2}\begin{cases} 1, & l=0,\quad m=m' \\ [i\pi(lN+m'-m)]^{-1} & \text{otherwise.}\end{cases} \qquad (2.21)$$

Now, we would like[1-3] to neglect in (2.20) all the terms with $l \neq 0$. If we could do so, we could use (2.6) for $B_0^{n,n'}$ and get, for I,

$$I = \sum_{m'} G_{nm'}\,\bar{U}(m'-m) . \qquad (2.22)$$

This is called by Zak and Zawadski[3] a "diagonal potential,"—diagonal, of course, in the sense that contributions to I come only from intraband terms. In order to go from (2.20) to (2.22), a sufficient (although not by all means necessary) condition is the following:

(a) Solve (2.18) only for small m's. We will have to show later that we need mostly terms of this kind.

(b) Assume $G_{n'm'}$ for small m's (small compared with N) to be much bigger with respect to those G's for larger m''s, so that we need to sum in (2.20) only on small m's. [It is worthwhile to mention that it is not enough to demand that $\bar{U}$ be small for large arguments as, for example, the term with $m'-m = -(n-1)$, $l=1$, though "nondiagonal," is big.]

(c) Under conditions (a), (b), i.e., for small m, m', demand

$$\sum_{l\neq 0} B_l^{nn'}\,\bar{U}(lN+m'-m) \ll B_0^{nn'}\,\bar{U}(m'-m) . \qquad (2.23)$$

$B_l^{nn'}$, being Fourier coefficients of continuous differentiable functions (2.16), decrease asymptotically at least[10] as $1/l$. Thus if $\bar{U}(p)$ goes asymptotically not slower than $1/p$, we need concern ourselves only with a finite summation in (2.23). We assume (and this should in principle be checked for each case) that the $B_l^{nn'}$ do not rise too rapidly for small l ($\neq 0$). Then, in order that (2.23) exist, we need

$$\bar{U}(lN+m'-m) \ll \bar{U}(m'-m), \qquad l\neq 0,\quad |m-m'| \ll N . \qquad (2.23')$$

In our case

$$\frac{\bar{U}(lN+p)}{\bar{U}(p)} \approx \frac{1}{lN} , \text{ (for small } p)$$

by (2.21), so that, unless $B_l^{nn'}$ rises in this manner (which we assume is not the case), condition (c) is fulfilled. We will discuss conditions (a) and (b) below.

With these assertions, (2.18) gets the form (compare Refs. 1–3)

$$\sum_{n'm'} (H^{(0)} + H^{(1)} + Q)_{nm,n'm'}\,G_{n'm'} = \epsilon\,G_{nm} , \qquad (2.24)$$

where

$$H^{(0)}_{nm,n'm'} = \left[\epsilon_n^{(0)} + \frac{\hbar^2}{2M}\left(\frac{2\pi m}{L}\right)^2\right]\delta_{nn'}\,\delta_{mm'}\,,$$

$$H^{(1)}_{nm,n'm'} = \frac{\hbar}{M}\,\frac{2\pi m}{L}\,p_{nn'}\,\delta_{mm'}\,, \qquad (2.25)$$

$$Q_{nm,n'm'} = \overline{U}(m'-m)\delta_{nn'}\,.$$

The nondiagonal terms in $H^{(1)}$ are of the order of $2\pi/L$. Since in the EMA one retains terms up to the order $(2\pi/L)^2$ (the approximation being no longer valid for higher-order terms), we would like to transform them away. These elements can be eliminated to a first order in $2\pi/L$ by the transformation[1] [which stays with the same m, so that (a), (b) are not affected]

$$G = e^{S}D; \quad S_{nm,n'm'} = \begin{cases} -\dfrac{\hbar}{M}\,\dfrac{2\pi m}{L}\,\dfrac{p_{nn'}}{w_{nn'}}\,\delta_{mm'}\,, & n \neq n' \\ 0, & n = n' \end{cases} \qquad (2.26)$$

where $w_{nn'} = \epsilon_n(0) - \epsilon_{n'}(0)$. We note that this transformation does not depend on the particular auxiliary potential, but only on the unperturbed Bloch problem. The correction terms to Q coming from this transformation [see Eq. (2.33) of Ref. 1] are

$$\langle nm \mid [QS] \mid n'm' \rangle = \frac{\hbar}{M}\,\frac{2\pi}{L}\,(m-m') \times \frac{p_{nn'}}{w_{nn'}}\,\overline{U}(m-m'), \qquad n \neq n' \quad (2.27)$$

where again we have used (2.23). The order of these interband terms is again [like $H^{(1)}$ in (2.25)] $2\pi/L$. It seems therefore that in order to get rid of the interband terms of $H^{(1)}$ we have created new interband elements of the same order. However,[1] these matrix elements can be neglected with respect to those which are retained in the EMA provided the additional coefficient multiplying them [namely, $\overline{U}(m-m')/w_{nn'}$] is small. Recalling that this comes in squared (being a part of interband elements), we impose the following condition for the EMA to be valid:

$$\overline{\overline{U}}(p)/w < 1\,,$$

where $\overline{\overline{U}}(p)$ is a typical Fourier component of $U(x)$ (for small p), while w is the energy gap. In our case, by (2.21), $\overline{\overline{U}}(p)$ is of the order of $eV/2\pi$, where V is the potential difference on the crystal. Thus we have a strict criterion for the applicability of the EMA for this *finite* problem, namely, that the potential difference (in energy units) be smaller than the energy gap,

$$V < \epsilon_g\,. \qquad (C\,1)$$

This is a most important result, stressing the importance of the voltage differences on the sample (or perhaps on a mean free path in scattering cases). Again, this criterion shows why the EMA is not valid for infinite crystals. With these provisions we get as an equation for $\{D\}$, (2.26):

$$\overline{\epsilon}_n(m)D_{nm} + \sum_{m'}\overline{U}(m'-m)D_{nm'} = \epsilon D_{nm}\,, \qquad (2.28)$$

where $\overline{\epsilon}_n(m)$ is understood to be the development of $\epsilon_n(m)$ to second order in $2\pi/L$. Now, for each n we have N D's ($m = 0, 1, \ldots, N-1$). We define a function F_n which is given originally only on the discrete points la, $l = 0, 1, \ldots, N-1$:

$$F_n(l) = \sum_{m=0}^{N-1} D_{nm}\,e^{i2\pi lam/L}\,. \qquad (2.29)$$

The energy $\epsilon_n(m)$ can be taken to be periodic in m with a period N, $\epsilon(m+N) = \epsilon(m)$, and then can be developed in Fourier series with only N terms:

$$\epsilon_n(m) = \sum_{l=0}^{N-1} E_n^{\,l}\,e^{-i2\pi lm/N}\,. \qquad (2.30)$$

Multiply (2.28) by $e^{i2\pi lm/N}$ and sum over m. The first term becomes

$$\sum_{mm'} E_n^{\,m'}\,D_{nm}\,e^{i2\pi m(l-m')/N} = \left[\sum_{m'} E_{nm'}\,T(-m')\right]F_n(l)\,, \qquad (2.31)$$

which has the effect of operating on $F_n(l)$ by an operator $\hat{\epsilon}_n$ which is built from $\epsilon_n(m)$ by replacing $2\pi m/N$ by $\partial/\partial x$, leading to the translation operators T. The second term of (2.28) becomes

$$\sum_{m'm}\overline{U}(m'-m)D_{nm'}\,e^{i2\pi lm/N} = \sum_{p=m'-N+1}^{m'}\sum_{m'}\overline{U}(p)e^{-i2\pi lp/L}D_{nm'}\,e^{i2\pi lm'/N}\,.$$

If we assume again the sum over m' to contain only small m', and $U(x)$ to be given by a small number of Fourier terms, we have for the latter approximately $U(la)F_n(l)$, and thus (2.1) goes into

$$[\hat{\epsilon}_n + U(la)]F_n(l) = \epsilon\,F_n(l)\,, \qquad (2.32)$$

which is the EMA operation.

Equation (2.32) is a difference[2] equation and not a differential one. No conscientious effort has been made to date to justify using the derived differential equation[11] instead of (2.32). Now, considering condition (b) above, we see that in order for it to be valid the D_{nm}'s for small m's must be much bigger than those with large m's [the transformation (2.26) has only a negligible effect]. This means[3] that F_n, the solution of (2.32), has to have mostly "small m" Fourier components [see Eq. (2.29)].

Thus there is a restriction on the ability to use the EMA (as was commented upon in Ref. 3). In our case, the $F_n(x)$ are solutions of Airy-type equations.[12] These functions (Airy functions[13]) have the following features: For $\epsilon < eEx$, the function is concave, with no zeros, while for $\epsilon > eEx$, the function is convex and there are oscillations, the number of nodes increasing with energy from 0 to $N-1$ in the interval $[0-L]$. The expressions we want to estimate are

$$D_{nm} = \frac{1}{N} \sum_{l=0}^{N-1} F_n(l)\, e^{-i2\pi lm/N} . \tag{2.33}$$

The node-free part of F does not pose great difficulties. A relatively small number of Fourier components is sufficient to represent it. To estimate the number of coefficients needed for the oscillating part, we calculate the smallest "period" of the function and demand that the wavelength of the highest Fourier term (m_{mx}) be smaller than that. In order to fulfill condition (b) this m_{mx} has to be small compared to N. But N in real crystals is a large number (of the order of 10^7). Now the larger the number of nodes of F, the larger is the number of the Fourier components needed for its development. It is therefore necessary to consider only those functions (belonging to higher energy levels) having a large (with respect to 1) number of nodes (but still small, of course, compared to N). The number of nodes in the interval $[0, L]$ depends on the energy level in the band n. If we denote the levels by the number p beginning at the lower edge of the band, the first level ($\epsilon_{n,1}$) has no nodes, $\epsilon_{n,2}$ has one node, etc. Thus, the number of nodes for $F_{n,p}$ is $p-1$. As will be seen below, the distance between nodes decreases with the function's argument $|Z|$. Hence only the farthest (away from $Z=0$) negative arguments will be considered. For the functions we consider, namely, those having a large number of zeros, we can use their asymptotic expansions which are[12,13]

$$F_{n,p}(-Z) \simeq \frac{C}{Z^{1/4}} \sin(\tfrac{2}{3} Z^{3/2} + \tfrac{1}{4}\pi) , \tag{2.34}$$

where

$$Z = \alpha^{1/3} x - \frac{\epsilon'_{n,p}}{\alpha^{2/3}} ,$$

$$\epsilon'_{n,p} = \frac{2m^* \epsilon_{n,p}}{\hbar^2} , \quad \alpha = \frac{2m^* eE}{\hbar^2} ,$$

and m^* is the effective mass.

The "period" of oscillation of F is seen from (2.34) to decrease with $|Z|$, the smallest being that one near the $(p-1)$th node. It can be calculated from (2.34) by, say, finding the interval between two successive zeros of F. These zeros occur for $Z = (\frac{3}{2}\pi\nu)^{2/3}$, where ν is an integer, $\nu = 0, 1, 2, \ldots, (p-1)$. The smallest interval between successive nodes for x is (for $p \gg 1$) $\Delta x_p = \pi^{2/3} \times (2/3\alpha p)^{1/3}$, which is one-half of the wavelength. The wavelength of the mth Fourier term in the sum (2.33) is $\lambda_m = Na/m$. In order that the Fourier sum be a good representation for F, we need $\lambda_{m_{mx}} < \Delta x_p$, or

$$m_{mx} > Na(3\alpha p)^{1/3}/2^{1/3}\pi^{2/3} . \tag{2.35}$$

Now, in order to use the EMA, this m_{mx} should be smaller than N, i.e.,

$$p < \tfrac{2}{3} E_k / v , \tag{C 2}$$

where

$$E_k = \frac{\hbar^2}{2m^*} \left(\frac{\pi}{a}\right)^2$$

is the kinetic energy of a free particle in the edge of the Brillouin zone and $v = eEa$ is the potential energy drop on one unit cell. This establishes a second condition for the validity of the EMA. It means that we can use the EMA for a part of the band only. Let us write (C 2) in another form. Recalling[12] that the energy levels of the "empty lattice" in the presence of the constant electric field are given by

$$\epsilon_p = \frac{\hbar^2}{2m^*} \left(\frac{3\pi}{2}\, \alpha p\right)^{2/3} \tag{2.36}$$

for $p > 1$, the above condition can be put in the form

$$\epsilon_p < E_k . \tag{C 2'}$$

The smallest distance from a *band edge* of the last energy level for which the EMA can be used has to be smaller than the kinetic energy of a free electron in the edge of the Brillouin zone. To get a feeling for this criterion we calculate it for a specific example. For a of the order 5 Å we get $E_k \approx 1$ eV. v is given by $5\times10^{-4}E$ (eV) when E is measured in 10^4 V/cm. Thus the criterion for this case is

$$p < 10^3/E \ (E \text{ in units of } 10^4 \text{ V/cm}) ,$$

which even for high electric fields has a relatively high upper bound for p.

III. DISCUSSION

Two conditions were obtained for the validity of the EMA for crystals in finite-range electric fields, namely, (C 1) and (C 2). Condition (C 1) restricts greatly the possibility of using the EMA particularly for an explanation of the electro-optic absorption experiments hitherto performed.[14] These experiments were usually carried out with voltages much higher for the specimens used than that allowed by (C 1). However, for thin enough samples one can have very strong fields and still fulfill (C 1). A calculation which has been carried out for the

electro-optic absorption using the EMA will appear in a future publication.[15] Some changes from the present results (obtained using the Franz-Keldish theory) have been calculated.[15] It might be possible that one could use a less-strict condition by considering L as the mean free path in a crystal instead of its length. This matter is now under investigation. The second condition (C 2) restricts the range of energy for which the EMA can be applied. It has a simple form and can easily be checked. A similar criterion appears for the impurity problem[3] and for the case of a crystal in a constant magnetic field.[4] In the case of a constant magnetic field, however, this restriction is usually ignored in calculating the optical magnetoabsorption.[16] The condition (C 2) gives also a better qualitative understanding why the EMA cannot be used for the case of an infinite crystal in a constant electric field: It is clear that as the number of nodes of the eigenfunctions increases, the smallest "period" decreases (see the expression for Δx_p above) and the number of Fourier terms needed to represent the function increases. For an infinite crystal, this "period" goes to zero and thus the function cannot be developed in a finite number of terms anymore.

Let us stress again that while for the infinite crystal there is no justification to use the EMA, this approximation was shown to *be* applicable to real (finite) crystals under conditions (C 1) and (C 2).

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Surface-Plasmon Dispersion: A Comparison of Microscopic and Hydrodynamic Theories*†

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The hydrodynamic theory of the electron gas, first applied to surface plasmons in metals by Ritchie, is critically examined using the equation of motion for the Wigner distribution function in the random-phase approximation (RPA). It is found that the theory does not agree with the RPA in the case of surface plasmons, though it does for bulk plasmons.

I. INTRODUCTION

In deriving the dispersion relation of surface plasmons in metals, several authors[1-3] have used the hydrodynamical equations for a charged fluid. While one may view with some suspicion the application of these equations to the so-called "collisionless" region, it is nevertheless true that the wave-vector dependence of the bulk-plasmon frequency, calculated by the hydrodynamic theory, is in apparent agreement with the prediction of the random-phase approximation (RPA),[4] to the lowest order