Deformation potentials in 2D- and 3D-deformable jellium

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Abstract. This paper gives an analysis of the dependence of the strength of the deformation potential on the dimensionality of the solid. The model chosen to represent the electron gas interacting with the background of ions is the 2D- and 3D-deformable jellium. It is shown that the strength of the deformation potential in 2D-deformable jellium is higher than that in the 3D case.

1. Introduction

The rôle of deformation potential in semiconductor physics has received much attention, both theoretically [1–18] and experimentally [19–24], since Bardeen and Shockley [1] introduced the concept in 1950 in the context of electron–phonon coupling in semiconductors. The concept has been generalized and extended to more complicated systems including general strain effects in metals and dielectrics [2–10]. Parmenter [2] gave a method of evaluating deformation potentials using a modified perturbation theory, rather than the conventional first-order perturbation theory. Later, perturbation-theoretic methods using an inverse transformation of coordinates between the strained and the unstrained systems, so as to use the same boundary conditions in the two cases, were developed further by Whitfield [7], by Bir and Pikus [5], and by Kartheuser and Rodriguez [14]. The effect of the long-range electrostatic contribution on the deformation potentials was taken into account by Lawaetz [15], Gram and Jørgensen [16], Resta and co-workers [17, 18], and Van de Walle and Martin [25]. Recently, more rigorous and more general proofs of the deformation potential theorem (i.e., the relation between the matrix elements of the electron–phonon interaction and the shifts of the electronic levels as a function of macroscopic strain) have been provided by Khan and Allen [12] for the rigid-ion model, by Kartheuser and Rodriguez [14] for both rigid-ion and deformable-ion models, and by Resta [18] within the framework of density-functional theory.

There have been some discussions lately on the deformable jellium model [26]. In the ordinary jellium model of a homogeneous electron gas the positive background is non-responsive, providing local charge neutrality only in equilibrium. In the case of low electron density, when the electronic part of the system develops long-range order (e.g., charge-density waves or Wigner solid), it is instructive to consider a deformable jellium [26] in which the background shows its response by deforming itself to preserve local charge neutrality, so that the long-range Coulomb interaction is diminished. Therefore, there are no long-range electrostatic contributions to deformation potentials in the deformable jellium. The evaluation of deformation potentials is done from the change in electronic

 4897

band parameters caused by strain and the consequent change in the lattice constants of the crystal. When the strain is due to acoustic waves of long wavelength, the background can be well approximated by a continuum as in the deformable jellium model.

Deformation potentials play a major rôle in the properties of carrier mobilities [3–5, 23], acoustoelectric effect [19], cyclotron resonances [20], piezo-electroreflectance [21], electron–phonon interaction [13, 22], phonon emissions [24, 27], absorption of heat pulses [28], band line-up in semiconductor heterojunctions [25], etc. There are several different definitions of deformation potential depending on the kinds of strain applied to the system [1, 4] and the energy states compared before and after the deformation [12–14]. Furthermore, there is some confusion in terminology [29] and definition of deformation potentials [30].

This work deals with deformation potentials in a deformable jellium where the density parameter (r_s) is less than that at the melting point of the Wigner crystal. We shall deal with the hydrostatic deformation potential associated with hydrostatic strains. The Rydberg (Ryd) is the unit of energy and of the deformation potential used in the paper. Most calculations for low-dimensional systems of physical quantities that depend on the deformation potential have used the 3D results. To our knowledge, *ab initio* estimates of the deformation potential of a 2D system have not been made before.

We compare the energy of 2D- and 3D-deformable jellium in section 2. We shall give a brief discussion of the several definitions of deformation potentials and the relations between them and provide exact expressions of the hydrostatic deformation potentials in 2D- and 3D-deformable jellium within the Hartree–Fock (HF) approximation in section 3. Section 4 gives a brief summary.

2. Hamiltonian for a deformable jellium in the HF approximation

The jellium model [31] consists of a system of N electrons embedded in a homogeneous background of equal positive charge so that the system is electrically neutral. The jellium Hamiltonian $\mathcal{H}$ may be written as

$$\mathcal{H} = -\frac{\hbar^2}{2m}\sum_i \nabla_i^2 + \sum_{i<j}\frac{e^2}{|r_i - r_j|} + V_{bb} + V_{eb} \tag{2.1}$$

where V_{bb} and V_{eb} are the background–background interaction and the electron–background interaction respectively. In the HF approximation, the Hamiltonian can be written as

$$\mathcal{H}_{HF} = T + V_d + V_{ex} + V_{bb} + V_{eb} \tag{2.2}$$

where T is the kinetic energy, and V_d and V_{ex} are the direct and non-local exchange parts of the electron–electron interaction respectively. The deformable jellium is defined by the condition [26]

$$V_d + V_{bb} + V_{eb} = 0 \tag{2.3}$$

which means that the positive background deforms itself in order to locally neutralize the system. In this deformable jellium, the single-particle energy $\varepsilon(k)$ can be written in terms of the kinetic energy and exchange energy parts:

$$\mathcal{E}(k) = t(k) + v_{ex}(k) \tag{2.4}$$

where

$$t(k) = \left\langle \psi_k(r) \left| -\frac{\hbar^2}{2m}\nabla^2 \right| \psi_k(r) \right\rangle \tag{2.5}$$

$$v_{\text{ex}}(k) = -\sum_{k_1(\text{occ})} \left\langle \psi_k(r_1)\psi_{k_1}(r_2) \left| \frac{e^2}{|r_1 - r_2|} \right| \psi_k(r_2)\psi_{k_1}(r_1) \right\rangle. \tag{2.6}$$

Let us consider a deformable jellium in which the electron density parameter (r_s) is less than the melting point of the Wigner crystal. In this case, we use plane waves as solutions in an approximation [26]. In the 3D-deformable jellium, the plane wave function $\psi_k(r) = (1/\sqrt{\Omega_0})\, e^{ik\cdot r}$, with normalization volume Ω_0, gives the energy eigenvalue from equations (2.4), (2.5), (2.6) as [32]

$$\mathcal{E}^{3D}(\eta, r_s) = (9\pi/4)^{2/3}(\eta/r_s)^2 - (4/\pi)(9\pi/4)^{1/3}\,(1/r_s)\,F(\eta)$$
$$F(\eta) = \left[\tfrac{1}{2} + [(1 - \eta^2)/4\eta] \ln |(1 + \eta)/(1 - \eta)|\right] \tag{2.7}$$
$$r_0 = (3/4\pi\rho)^{1/3} = (9\pi/4)^{1/3}/k_F$$
$$r_s = r_0/a_0 \qquad \eta = k/k_F$$

where ρ is the volume density of the electrons, k_F is the Fermi wave vector, r_0 is the Wigner–Seitz radius, r_s is the density parameter, and a_0 is the Bohr radius.

In the 2D-deformable jellium, the wave function of the state with wave vector k is

$$\psi_k(R) = \frac{1}{\sqrt{A_0}} e^{ik\cdot R} \tag{2.8}$$

where R is the 2D position vector, k is the 2D wave vector, and A_0 is the area for normalization. The exchange energy of one electron with wave vector k [33] is

$$v_{\text{ex}}^{2D}(k) = -e^2 \sum_{k_1(\text{occ})} \left\langle \psi_k(R_1)\psi_{k_1}(R_2) \left| \frac{1}{|R_1 - R_2|} \right| \psi_k(R_2)\psi_{k_1}(R_1) \right\rangle$$
$$= -\frac{2e^2 k_F}{\pi} \mathbb{E}\left(\frac{k}{k_F}\right) \tag{2.9}$$

where $\mathbb{E}(x) = E(\pi/2, x) = \int_0^{\pi/2} \sqrt{1 - x^2\sin^2\theta}\, d\theta$ is a complete elliptic integral of the second kind. Therefore, the energy eigenvalue in 2D-deformable jellium is given by

$$\mathcal{E}^{2D}(\eta, r_s) = 2(\eta/r_s)^2 - (4\sqrt{2}/\pi)\,(1/r_s)\,\mathbb{E}(\eta)$$
$$r_0 = (1/\pi n)^{1/2} = \sqrt{2}/k_F \tag{2.10}$$
$$r_s = r_0/a_0 \qquad \eta = k/k_F$$

where n is the areal density of the electrons and k_F is the Fermi wave vector in 2D.

Figure 1(a) shows the energy eigenvalues of an electron in 2D- and 3D-deformable jellium. There are big differences between the band structures for high density (small r_s), while there are slight differences between them for low density (large r_s). The energy eigenvalues of the quasiparticles in deformable jellium in 3D and 2D respectively are $\mathcal{E}^{3D}(0, r_s) = -(4/\pi)(9\pi/4)^{1/3}\,(1/r_s)$ and $\mathcal{E}^{2D}(0, r_s) = -2\sqrt{2}\,(1/r_s)$ at $k = 0$, and $\mathcal{E}^{3D}(1, r_s) = (9\pi/4)^{2/3}(1/r_s)^2 - (2/\pi)(9\pi/4)^{1/3}\,(1/r_s)$ and $\mathcal{E}^{2D}(1, r_s) = 2(1/r_s)^2 - (4\sqrt{2}/\pi)\,(1/r_s)$ at the Fermi surface $(k = k_F)$. Therefore, the exchange energy effect for 2D at the band minimum is stronger than that for 3D. In the ground state, the quasiparticle energies are always negative for $r_s > 3.015$ in 3D and for $r_s > 1.111$ in 2D.

The total energy can now be calculated from

$$E_{\text{total}} = 2\sum_k t(k) + \sum_k v_{\text{ex}}(k). \tag{2.11}$$
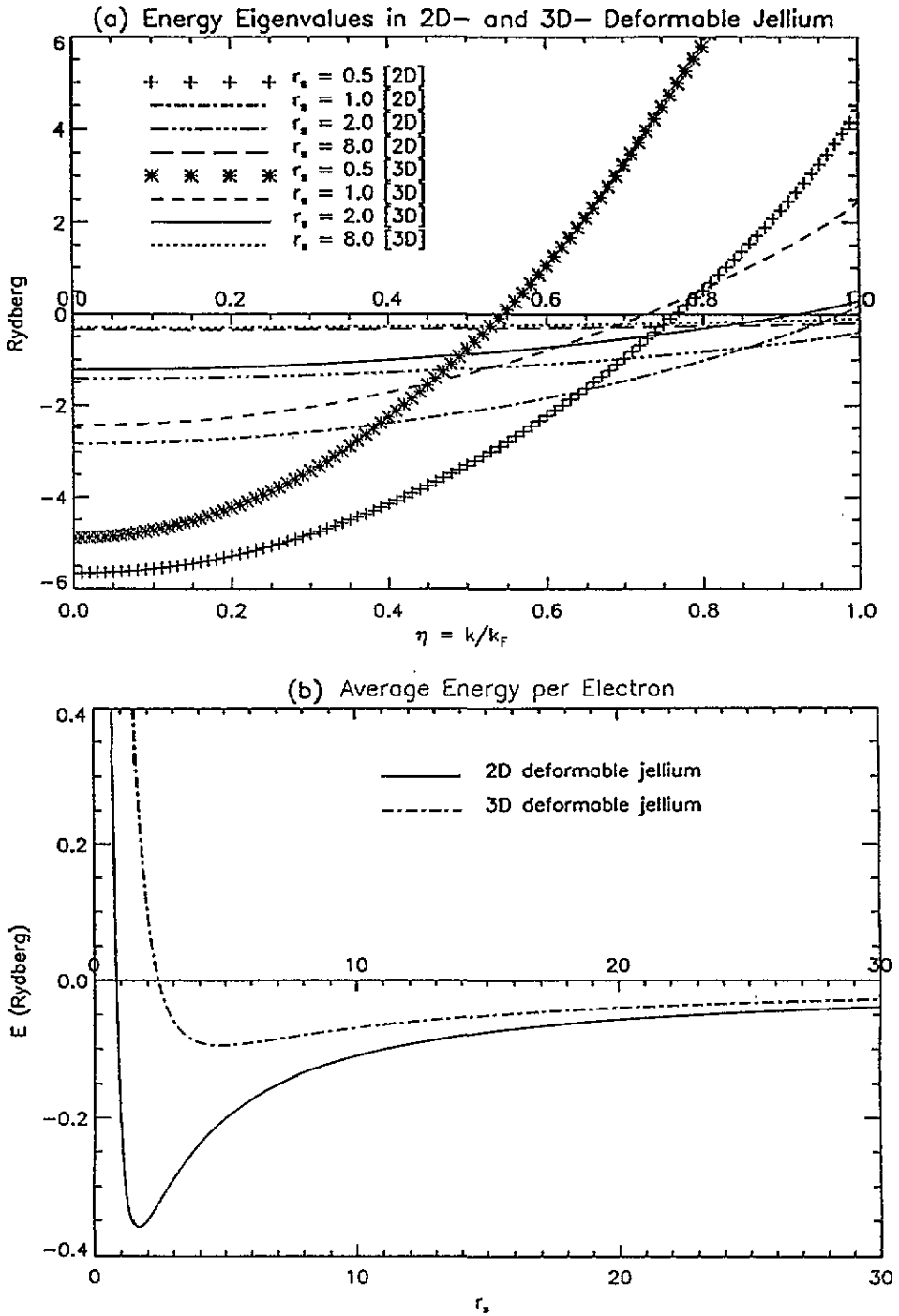
Figure 1. Comparisons of (a) the energy eigenvalues of an electron as a function of $\eta = k/k_F$ and (b) the average energy per electron in deformable jellium with respect to the electron density parameter r_s.

Therefore, the average energy of an electron in 2D- and in 3D-deformable jellium can be derived from equations (2.7), (2.10), (2.11):

$$\mathcal{E}_{ave}^{2D}(r_s) = \frac{1}{r_s^2} - \frac{8\sqrt{2}}{3\pi}\frac{1}{r_s} \tag{2.12}$$

$$\mathcal{E}_{ave}^{3D}(r_s) = \frac{3}{5}\left(\frac{9\pi}{4}\right)^{2/3}\frac{1}{r_s^2} - \frac{3}{2\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s}. \tag{2.13}$$

As shown in figure 1(b), while the average energy per electron in 2D differs significantly from that in 3D for high density, the average energy per electron for low density is similar for the two dimensions. The minima of the average energy per electron with respect to r_s in 2D and 3D are -0.360 Ryd at $r_s = 1.67$ and -0.095 Ryd at $r_s = 4.82$ respectively. The average energy per electron in 2D is more sensitive than that in 3D with respect to the electron density parameter r_s. The average energy per electron is always negative in the range of $r_s > 0.83$ in 2D and $r_s > 2.41$ in 3D.

3. Effect of strain on energy eigenvalues

Let us first consider the effect of a general external macroscopic strain $\underline{\varepsilon}$ on the energy eigenvalues in deformable jellium. A general strain for small deformations is defined by [34]

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j}\right) \tag{3.1}$$

where u_i is the x_i-axis component of the displacement vector u. Even though we do not have any periodic structure of positive ions in a jellium, we can define a strain tensor of equation (3.1) along the lines of the theory of elasticity in continuous media [34].

There are several definitions of deformation potentials. Before classifying the deformation potentials, we first consider the effect of a strain on energy eigenvalues in a deformable jellium. The Schrödinger equation for an electron in an unstrained deformable jellium is

$$[H_0(r, \nabla, \psi_{k_1})\psi_k] \equiv -\frac{\hbar^2}{2m}\nabla^2\psi_k(r)$$
$$-e^2\sum_{k_1}\int_{\Omega_0}\frac{\psi_{k_1}^*(r_1)\psi_k(r_1)}{|r - r_1|}\,\mathrm{d}r_1\,\psi_{k_1}(r) = \mathcal{E}^0(k)\psi_k(r) \tag{3.2}$$

with $\mathcal{E}^0(k) = t^0(k) + v_{ex}^0(k)$ and $\psi_k(r) = (1/\sqrt{\Omega_0})e^{ik\cdot r}$. The wave vector in the unstrained deformable jellium is given by

$$k_i = \frac{2\pi n_i}{L_i^0} \qquad (i = x, y, z; n_i = 0, \pm 1, \pm 2, \ldots) \tag{3.3}$$

where L_i^0 is the size of the unstrained system $(\Omega_0 = L_x^0 L_y^0 L_z^0)$. The Schrödinger equation for an electron in the strained deformable jellium can be written as

$$[H(r, \nabla, \psi_{k_{1\varepsilon}})\psi_{k_\varepsilon}] \equiv -\frac{\hbar^2}{2m}\nabla^2\psi_{k_\varepsilon}(r)$$
$$-e^2\sum_{k_{1\varepsilon}}\int_{\Omega_\varepsilon}\frac{\psi_{k_{1\varepsilon}}^*(r_2)\psi_{k_\varepsilon}(r_2)}{|r - r_2|}\,\mathrm{d}r_2\,\psi_{k_{1\varepsilon}}(r) = \mathcal{E}(k_\varepsilon)\psi_{k_\varepsilon}(r) \tag{3.4}$$

where $\mathcal{E}(k_\varepsilon) = t(k_\varepsilon) + v_{ex}(k_\varepsilon)$ is the single electron energy and $\psi_{k_\varepsilon}(r) = (1/\sqrt{\Omega})e^{ik_\varepsilon \cdot r}$ is the eigenfunction in the strained deformable jellium. If the eigenstate in the unstrained deformable jellium has a wave vector k, the corresponding eigenstate in the strained deformable jellium has the wave vector $k_\varepsilon = (\underline{1} - \underline{\varepsilon}) \cdot k$. The effect of a small strain $\underline{\varepsilon}$ may be treated as a perturbation. Introducing new coordinates such that [5]

$$r' = (\underline{1} + \underline{\varepsilon})^{-1} \cdot r = (\underline{1} - \underline{\varepsilon}) \cdot r \tag{3.5}$$

$$p' = (\underline{1} + \underline{\varepsilon}) \cdot p \tag{3.6}$$

the Schrödinger equation in the new coordinates, to within the first order of strain ε_{ij}, can be written as

$$[H'] = [H_0(r', \nabla', \psi'_{k_{1\varepsilon}})\psi'_{k_\varepsilon}] + \sum_{ij} \varepsilon_{ij} D_{ij}(r', \nabla', \psi'_{k_\varepsilon}, \psi'_{k_{1\varepsilon}})$$
$$= \mathcal{E}((\underline{1} - \underline{\varepsilon}) \cdot k'_\varepsilon)\psi'_{k_\varepsilon}((\underline{1} + \underline{\varepsilon}) \cdot r') \tag{3.7}$$

with

$$[H_0(r', \nabla', \psi'_{k_{1\varepsilon}})\psi'_{k_\varepsilon}] \equiv -\frac{\hbar^2}{2m}\nabla'^2 \psi'_{k_\varepsilon}((\underline{1} + \underline{\varepsilon}) \cdot r')$$
$$-e^2 \sum_{k_{1\varepsilon}} \int_{\Omega_0} \frac{\psi'^*_{k_{1\varepsilon}}((\underline{1} + \underline{\varepsilon}) \cdot r')\psi'_{k_\varepsilon}((\underline{1} + \underline{\varepsilon}) \cdot r')}{|r' - r'_1|} dr'_1 \psi'_{k_{1\varepsilon}}((\underline{1} + \underline{\varepsilon}) \cdot r') \tag{3.8}$$

and

$$[D_{ij}(r', \nabla', \psi'_{k_{1\varepsilon}})\psi'_{k_\varepsilon}] \equiv -\frac{\hbar^2}{m}\nabla'_i \nabla'_j \psi'_{k_\varepsilon}((\underline{1} + \underline{\varepsilon}) \cdot r')$$
$$+e^2 \sum_{k_{1\varepsilon}} \int_{\Omega_0} \frac{\psi'^*_{k_{1\varepsilon}}((\underline{1} + \underline{\varepsilon}) \cdot r'_1)(r' - r'_1)_i (r' - r'_1)_j \psi'_{k_\varepsilon}((\underline{1} + \underline{\varepsilon}) \cdot r'_1)}{|r' - r'_1|^3} dr'_1$$
$$\times \psi'_{k_{1\varepsilon}}((\underline{1} + \underline{\varepsilon}) \cdot r'). \tag{3.9}$$

In other words, the the energy eigenvalue of the strained deformable jellium in the new coordinates can be written as

$$\mathcal{E}((\underline{1} - \underline{\varepsilon}) \cdot k'_\varepsilon) = \mathcal{E}((\underline{1} - \underline{\varepsilon}) \cdot k) \tag{3.10}$$

because we have $k_\varepsilon = (\underline{1} - \underline{\varepsilon}) \cdot k'_\varepsilon$ from the coordinate transformation and $k_\varepsilon = (\underline{1} - \underline{\varepsilon}) \cdot k$ from the effect of the strain. Therefore, we have $k'_\varepsilon = k$. $[H]$ can now be regarded as a perturbation of $[H_0]$. The wave function of $[H_0(r', \nabla', \psi'_{k_{1\varepsilon}})\psi'_{k_\varepsilon}]$ is just the plane wave form $(1/\sqrt{\Omega_0})e^{ik \cdot r'}$. When it is written in terms of the original coordinates of the strained deformable jellium, the wave function is

$$\psi_k(r') = \frac{1}{\sqrt{\Omega_0}} e^{ik \cdot (\underline{1} - \underline{\varepsilon}) \cdot r}. \tag{3.11}$$

Therefore, ψ_k belongs to the wave vector $k_\varepsilon = (\underline{1} - \underline{\varepsilon}) \cdot k$ and to energy $\mathcal{E}^0(k_\varepsilon)$. The energy eigenvalue of $[H']$ associated with the solution of

$$[H_0(r', \nabla', \psi_{k_1}(r'))\psi_k(r')] \equiv \mathcal{E}^0(k)\psi_k(r') \tag{3.12}$$

is

$$\mathcal{E}((\underline{1} - \underline{\varepsilon}) \cdot k) = \mathcal{E}^0(k) + \sum_{ij} \varepsilon_{ij} \langle D_{ij} \rangle \qquad \langle D_{ij} \rangle = \int_{\Omega_0} \psi_k^*(r)[D_{ij}] \, dr. \tag{3.13}$$

There is no unique definition of the deformation potential for a strain $\underline{\varepsilon}$. If we compare the energies at the wave vector k_ε in the strained system and the wave vector k in the unstrained system, then the deformation potential [35] is given by

$$\Xi_{ij}^{bs}(k) = \lim_{\varepsilon_{ij} \to 0} \frac{\mathcal{E}((\underline{1} - \underline{\varepsilon}) \cdot k) - \mathcal{E}^0(k)}{\varepsilon_{ij}} = \langle D_{ij} \rangle \tag{3.14}$$

where $\langle D_{ij} \rangle = \langle k | D_{ij} | k \rangle$ and $\Xi_{ij}^{bs}(k)$ is called the band structure deformation potential [12–14]. If we compare the energies at the same value of k, the deformation potential is defined by

$$\Xi_{ij}^{x}(k) = \lim_{\varepsilon_{ij} \to 0} \frac{\mathcal{E}(k) - \mathcal{E}^0(k)}{\varepsilon_{ij}} = \frac{1}{2} \left[k_i \frac{\partial \mathcal{E}^0}{\partial k_j} + k_j \frac{\partial \mathcal{E}^0}{\partial k_i} \right] + \langle D_{ij} \rangle. \tag{3.15}$$

Suppose now that there is a phonon with a wave vector q. The displacement u at the point r gives rise to a change in the density of the electrons. Hence the change of density induces a change in potential (i.e. $\delta V(r) = V(r - u) - V(r) = \sum_{ij} V^{ij} \varepsilon_{ij}$). The deformation potential theorem introduced by Bardeen and Shockley [1] is the relation of the change per macroscopic strain in the energy of an electron level to the matrix elements of the electron–phonon interaction. The theorem for phonons with wave vector q is given by

$$\langle k + q | H_{ep} | k \rangle = \sum_{ij} \Xi_{ij}^{ep}(k) \varepsilon_{ij} = \sum_{ij} \left(\Xi_{ij}^{bs}(k) + m v_i(k) v_j(k) \right) \varepsilon_{ij} \tag{3.16}$$

where $H_{ep} = \delta V(r)$ is the change in the potential energy of an electron under the strain $\underline{\varepsilon}$ and $v_i(k)$ is the group velocity of the electron. The theorem was proved by Khan and Allen [12] within the rigid-ion model of $\delta V(r)$, by Kartheuser and Rodriguez [14] within both the rigid-ion model and the deformable-ion model of $\delta V(r)$, and by Resta [18] within the Kohn–Sham potential of $\delta V(r)$ in the density-functional theory. In fact, the theorems of [12, 14] are valid only for metals. Resta extended the theorem to both metals and dielectrics, which is valid for any long-wavelength phonon, by generalizing deformation potentials by taking into account the long-range nature of the Coulomb interaction which has a fourth-rank tensor term. He showed that the deformation potential theorem has different aspects in metals and dielectrics. In the case of deformable jellium, there is no effect of long-range Coulomb interaction, so that the deformation potential theorem is reduced to equation (3.16).

Let us now consider the deformation potentials due to kinds of strain applied to a 3D system. The hydrostatic deformation potential $\Xi_h(k)$ [1, 11] due to a uniform hydrostatic strain $\underline{\varepsilon}_h = \varepsilon_{xx} \hat{x}\hat{x} + \varepsilon_{yy} \hat{y}\hat{y} + \varepsilon_{zz} \hat{z}\hat{z}$ ($d \ln \Omega_0 = \text{Tr}(\underline{\varepsilon}) = 3\varepsilon$, $\varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{zz} = \varepsilon = dr_0/r_0$) is defined by

$$\Delta\mathcal{E}(k) = \Xi_b(k) \left(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} \right) = \Xi_{xx}(k)\varepsilon_{xx} + \Xi_{yy}(k)\varepsilon_{yy} + \Xi_{zz}(k)\varepsilon_{zz}. \tag{3.17}$$

The deformation potential $\Xi_d(k)$ [4] due to a dilation [29] $\underline{\varepsilon}_d = \varepsilon_{xx} \hat{x}\hat{x} + \varepsilon_{yy} \hat{y}\hat{y}$ ($d \ln A_0 = \varepsilon_{xx} + \varepsilon_{yy} = 2\varepsilon$), which is a strain of two directions perpendicular to one axis (e.g. z-axis) without a strain in the axis, is given by

$$\Delta\mathcal{E}(k) = \Xi_d(k) \left(\varepsilon_{xx} + \varepsilon_{yy} \right) = \Xi_{xx}(k)\varepsilon_{xx} + \Xi_{yy}(k)\varepsilon_{yy}. \tag{3.18}$$

And the deformation potential $\Xi_u(k)$ [4] due to a uniaxial strain $\underline{\varepsilon}_u = \varepsilon_{xx} \hat{x}\hat{x} + \varepsilon_{yy} \hat{y}\hat{y} + \varepsilon_{zz} \hat{z}\hat{z}$ ($\varepsilon_{xx} = \varepsilon_{yy} = -\sigma \varepsilon_{zz}$, σ is Poisson's ratio), which is a combination of a tension along an axis (e.g. z-axis) and a compression in the two directions perpendicular to the axis, is defined by

$$\Delta\mathcal{E}(k) = \Xi_u(k)\varepsilon_{zz} = \Xi_{xx}(k)\varepsilon_{xx} + \Xi_{yy}(k)\varepsilon_{yy} + \Xi_{zz}(k)\varepsilon_{zz}$$
$$= \left(-\sigma \left\{ \Xi_{xx}(k) + \Xi_{yy}(k) \right\} + \Xi_{zz}(k) \right) \varepsilon_{zz}. \tag{3.19}$$

It is easy to handle the uniaxial deformation potentials from the viewpoint of experiments [19–21].

In this work, we shall use the band structure deformation potential as given in equation (3.14) and the hydrostatic deformation potential as defined by equation (3.17). Therefore, the hydrostatic deformation potential in 3D can be written as

$$\Xi_h^{3D}(k) = \frac{1}{3}\sum_{i=1}^{3} \Xi_{ii}^{bs}(k) = \frac{1}{3}\sum_{i=1}^{3}\langle D_{ii}\rangle. \tag{3.20}$$

Let us define the hydrostatic deformation potential in 2D by

$$\Xi_h^{2D}(k) = \frac{1}{2}\sum_{i=1}^{2} \Xi_{ii}^{bs}(k) = \frac{1}{2}\sum_{i=1}^{2}\langle D_{ii}\rangle. \tag{3.21}$$

Also, we can define a uniaxial deformation potential in 2D due to a strain $\varepsilon_u^{2D} = \varepsilon_{xx}\hat{x}\hat{x} + \varepsilon_{yy}\hat{y}\hat{y}$ ($\varepsilon_{xx} = -\varsigma\varepsilon_{yy}$), which is a combination of an expansion along an axis (e.g. y-axis) and a compression along the other axis (e.g. x-axis), by

$$\Delta\mathcal{E}(k) = \Xi_u^{2D}(k)\varepsilon_{yy} = \Xi_{xx}(k)\varepsilon_{xx} + \Xi_{yy}(k)\varepsilon_{yy} = (-\varsigma\Xi_{xx}(k) + \Xi_{yy}(k))\varepsilon_{yy}. \tag{3.22}$$

The uniaxial deformation potential in both 2D (for $\varsigma = 1$) and 3D (for $\sigma = \frac{1}{2}$) should vanish for an isotropic band structure.

In the case of the 2D-deformable jellium, the hydrostatic deformation potential due to a uniform strain associated with $d\ln A_0 = \varepsilon_{xx} + \varepsilon_{yy} = 2\varepsilon$ ($\varepsilon = dr_0/r_0$) from equation (3.21) will be

$$\Xi_h^{2D}(r_s, \eta) = \frac{4\sqrt{2}}{\pi}\left(\frac{1}{r_s}\right)\mathbb{E}(\eta) - 2(\eta/r_s)^2. \tag{3.23}$$

In the 3D-deformable jellium, the hydrostatic deformation potential due to to a uniform strain associated with $d\ln\Omega_0 = 3\varepsilon = 3dr_0/r_0$ from equation (3.20) is

$$\Xi_h^{3D}(r_s, \eta) = \frac{4}{\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s}F(\eta) - \frac{2}{3}\left(\frac{9\pi}{4}\right)^{2/3}\left(\frac{\eta}{r_s}\right)^2. \tag{3.24}$$

As shown in figure 2, the kinetic energy contribution to the deformation potential is larger in the case of high electron density (for small r_s) than in that of low electron density (for large r_s) in both 2D and 3D. The deformation potential in 2D is generally higher than that in 3D for the same value of r_s (see figure 3). At the band minima, the deformation potentials are given by $\Xi_h^{2D}(r_s, 0) = 2\sqrt{2}(1/r_s)$ in 2D and $\Xi_h^{3D}(r_s, 0) = (4/\pi)(9\pi/4)^{1/3}(1/r_s)$ in 3D. Therefore, for the higher electron density, the deformation potential at the band minimum will also be higher. The quasiparticle deformation potential at the Fermi surface changes over from negative to positive value for increasing r_s at $r_s = 1.11$ for 2D and at $r_s = 2.01$ for 3D, and has maximum values, 0.41 Ryd at $r_s = 2.22$ for 2D, and 0.15 Ryd at $r_s = 4.02$ for 3D (see figure 3).

Let us now define the average deformation potential, which is the change of the average energy of an electron per uniform hydrostatic strain $d\ln S^{nD}(S^{2D} = A_0, S^{3D} = \Omega_0)$, by

$$\Xi_{ave}^{nD} = \frac{\Delta\mathcal{E}_{ave}^{nD}}{d\ln S^{nD}} = \frac{1}{n}r_s\frac{\partial\mathcal{E}_{ave}^{nD}}{\partial r_s} \tag{3.25}$$

where nD represents the dimension of the system and $\mathcal{E}_{ave}^{nD}$ is the average energy of an electron in dimension nD. Therefore, the average deformation potential in 2D-deformable jellium will be

$$\Xi_{ave}^{2D} = \frac{4\sqrt{2}}{3\pi}\frac{1}{r_s} - \frac{1}{r_s^2} \tag{3.26}$$

(a) Deformation Potentials in 2D Deformable Jellium

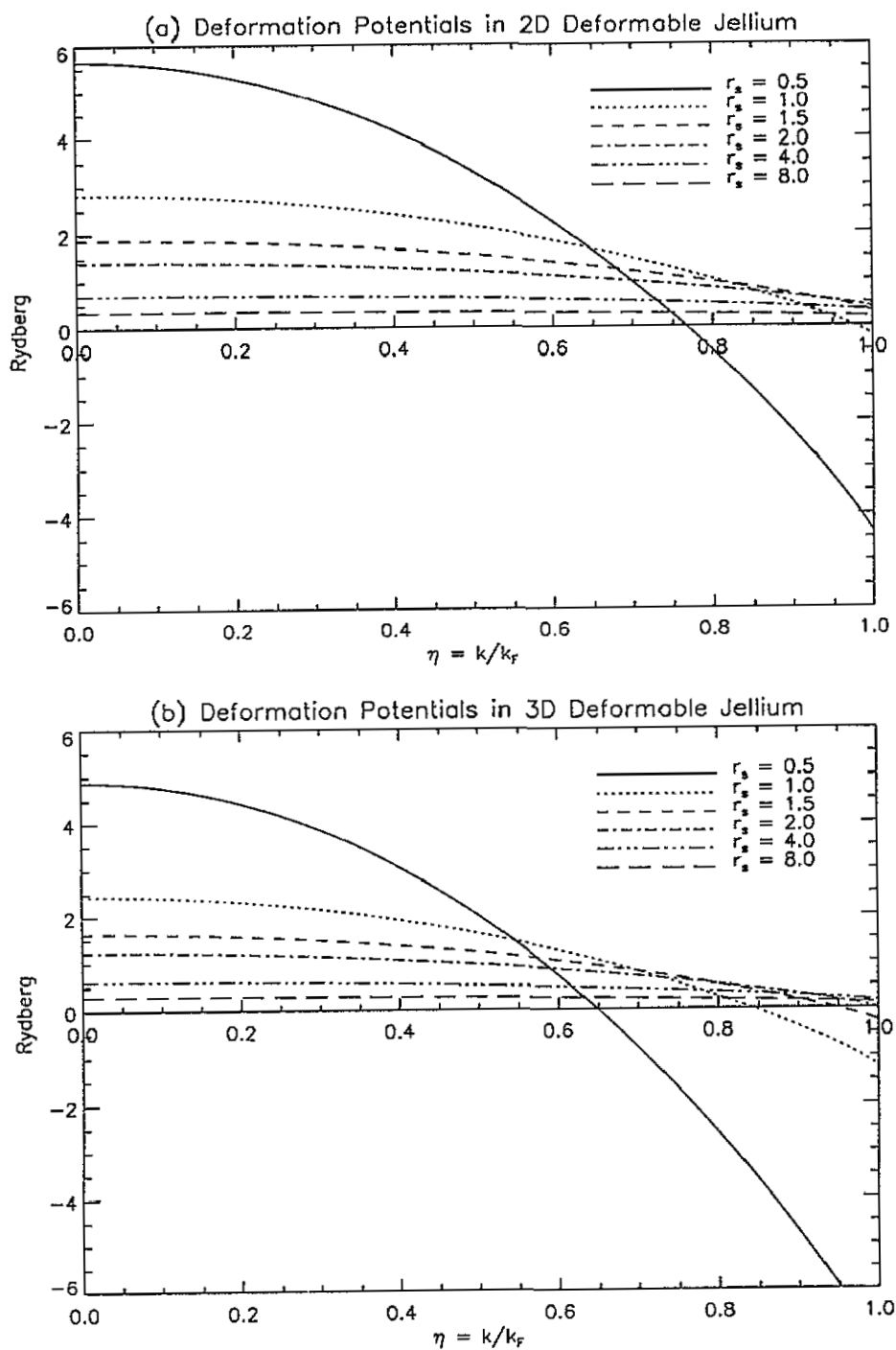**(b) Deformation Potentials in 3D Deformable Jellium**

Figure 2. The hydrostatic deformation potentials of a quasiparticle in (a) 2D-deformable jellium and (b) 3D-deformable jellium.

and the average deformation potential in the 3D-deformable jellium will be given by

$$\Xi^{3D}_{ave} = \frac{1}{2\pi} \left(\frac{9\pi}{4} \right)^{1/3} \frac{1}{r_s} - \frac{2}{5} \left(\frac{9\pi}{4} \right)^{2/3} \frac{1}{r_s^2}. \tag{3.27}$$
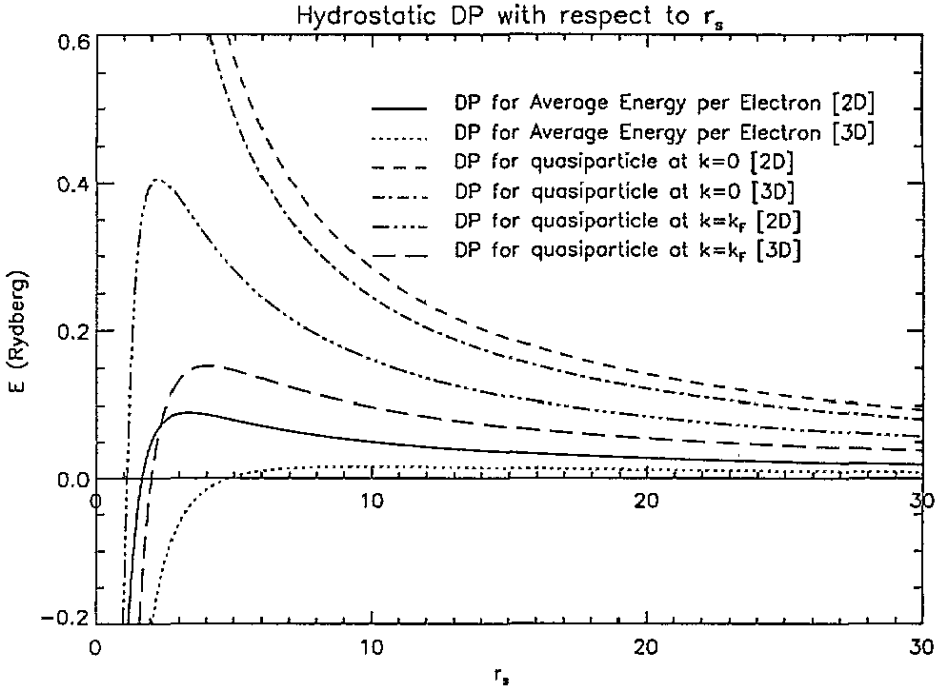
Figure 3. The hydrostatic deformation potentials (DP) for the quasiparticle energy and for the average energy per electron in deformable jellium with respect to the electron density parameter r_s.

The maximum of the average deformation potential is 0.090 Ryd at $r_s = 3.33$ in the 2D-deformable jellium and 0.016 Ryd at $r_s = 9.65$ in the 3D-deformable jellium (see figure 3). Neglecting the exchange part in 3D, while the average deformation potential Ξ^{3D}_{ave} is $-\frac{2}{5}\mathcal{E}_F$, the deformation potential Ξ^{3D}_h of a quasiparticle at the Fermi surface is given by $-\frac{2}{3}\mathcal{E}_F$, which was pointed out by Ziman [29]. In the 2D case, considering only the kinetic part, the average deformation potential Ξ^{2D}_{ave} is $-\frac{1}{2}\mathcal{E}_F$ and the deformation potential Ξ^{2D}_h of a quasiparticle at the Fermi surface is $-\mathcal{E}_F$.

4. Summary

It is established that the deformable jellium model provides a good description of the ground-state properties of many-particle metallic systems in the low-density regime. This model has been successfully applied [26] to electronically ordered states like charge-density-wave states and Wigner solids. Unlike ordinary jellium the deformable jellium includes the response of the background. The long-range Coulomb interactions are effectively screened by this response.

In this paper we have used the deformable jellium model to calculate the energy spectrum of quasi-particles in the HF approximation. Since we are away from any electronically ordered phase, we have used a plane wave as an approximation to the electronic states. Calculations of the quasi-particle energies are done for 2D- and 3D-deformable jellium. The quasi-particle energies are used to calculate the deformation potentials. It has been found that the strength of the deformation potential in 2D-deformable jellium is higher than that in the 3D case. We plan to extend this work to heterostructures with finite thickness.

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References

[1] Bardeen J and Shockley W 1950 *Phys. Rev.* **80** 72
[2] Parmenter R H 1955 *Phys. Rev.* **99** 1759, 1767
[3] Dumke W P 1956 *Phys. Rev.* **101** 531
[4] Herring C and Vogt E 1956 *Phys. Rev.* **101** 944
[5] Bir G L and Pikus G E 1974 *Symmetry and Strain-induced Effects in Semiconductors* (New York: Wiley)
Pikus G E 1958 *Sov. Phys.–Tech. Phys.* **3** 2194
[6] Pikus G E and Bir G L 1959 *Sov. Phys.–Solid State* **1** 1502
Bir G L and Pikus G E 1961 *Sov. Phys.–Solid State* **2** 2039
[7] Whitfield G D 1961 *Phys. Rev.* **121** 720
[8] Kleinman L 1962 *Phys. Rev.* **128** 2614
[9] Goroff I and Kleinman L 1963 *Phys. Rev.* **132** 1080
[10] Hasegawa H 1963 *Phys. Rev.* **129** 1029
[11] Vergés J A, Glötzel D, Cardona M and Andersen O K 1982 *Phys. Status Solidi* b **113** 519
[12] Khan F S and Allen P B 1984 *Phys. Rev.* B **29** 3341
[13] Khan F S and Allen P B 1987 *Phys. Rev.* B **35** 1002
[14] Kartheuser E and Rodriguez S 1986 *Phys. Rev.* B **33** 772
Rodriguez S and Kartheuser E 1985 *Superlatt. Microstruct.* **1** 503
[15] Lawaetz P 1969 *Phys. Rev.* **183** 730
[16] Gram N O and Jørgensen M H 1973 *Phys. Rev.* B **8** 3902
[17] Resta R, Colombo L and Baroni S 1990 *Phys. Rev.* B **41** 12358
[18] Resta R 1991 *Phys. Rev.* B **44** 11035
[19] Weinreich G, Sanders T M Jr and White H G 1959 *Phys. Rev.* **114** 33
[20] Hensel J C and Feher G 1963 *Phys. Rev.* **129** 1041
Murase K, Enjouji K and Otsuka E 1970 *J. Phys. Soc. Japan* **29** 1248
[21] See, e.g.,
Pollak F H and Cardona M 1968 *Phys. Rev.* **172** 816
[22] Lang I G and Pavlov S T 1971 *Sov. Phys.–Solid State* **12** 1926
Feyder G, Kartheuser E, Ram Mohan L R and Rodriguez S 1982 *Phys. Rev.* B **25** 7141
[23] Price P J 1985 *Phys. Rev.* B **32** 2643
Walukiewicz W, Ruda H E, Lagowski J and Gatos H C 1985 *Phys. Rev.* B **32** 2645
Vinter B 1986 *Phys. Rev.* B **33** 5904
[24] Rothenfusser M, Köster L and Dietsche W 1986 *Phys. Rev.* B **34** 5518
Toombs G A, Sheard F W, Neilson D and Challis L J 1987 *Solid State Commun.* **64** 577
[25] Van de Walle C G 1989 *Phys. Rev.* B **39** 1871
Van de Walle C G and Martin R M 1989 *Phys. Rev. Lett.* **62** 2028
[26] Overhauser A W 1968 *Phys. Rev.* **167** 691
Barrera R G, Grether M and de Llano M 1979 *J. Phys. C: Solid State Phys.* **12** L715
Méndez-Moreno R M, Ortíz M A and Moreno M 1989 *Phys. Rev.* A **40** 2211
Orozco S, Ortíz M A and Méndez-Moreno 1990 R M *Phys. Rev.* A **41** 5473
Méndez-Moreno R M and Moreno M 1990 *Phys. Rev.* A **41** 6662
Orozco S, Ortíz M A and Méndez-Moreno R M 1992 *Phys. Rev.* B **46** 13073
[27] Vass E 1987 *Solid State Commun.* **61** 127
Kent A J, Rampton V W, Newton M I, Carter P J A, Hardy G A, Hawker P, Russell P A and Challis L J 1988 *Surf. Sci.* **196** 410
Badalian S M and Levinson Y B 1991 *Phys. Lett.* **155A** 200
Hawker P, Kent A J, Hughes O H, and Challis L J 1992 *Semicond. Sci. Technol.* B **7** 29
[28] Hensel J C, Dynes R C and Tsui D C 1983 *Phys. Rev.* B **28** 1124
Hardy G A, Kent A J, Rampton V W and Challis L J 1989 *High Magnetic Fields in Semiconductor Physics II* ed G Landwehr (Berlin: Springer)
[29] In some papers (e.g. [1], [3], [8]), the dilation is used as the hydrostatic strain. Also, see
Ziman J M 1960 *Electrons and Phonons* (London: Oxford University Press)

Brooks H 1955 *Advances in Electronics and Electron Physics* ed L Marton (New York: Academic)

[30] In [5] (Pikus 1958), the sign of the deformation potential was taken to be opposite to the usual definition of deformation potential.

[31] See, e.g.,
      Inkson J C 1984 *Many Body Theory of Solids* (New York: Plenum) p 4

[32] See, e.g.,
      Madelung O 1978 *Introduction to Solid-State Theory (Springer Series in Solid State Science 2)* (Berlin: Springer)

[33] Stern F 1973 *Phys. Rev. Lett.* **30** 278
      Stern F 1974 *Proc. 2nd Int. Conf. on Solid Surfaces (Kyoto)*; *Japan. J. Appl. Phys. Suppl.* **2** 323
      The exchange energy of an electron with wave vector k in the extreme 2D limit of inversion layers was calculated by assuming no excited subbands exist. There are two types of definition of complete elliptic integrals, differing in their arguments. Stern's papers used the definition $E(x) = E(\pi/2, x) = \int_0^{\pi/2} \sqrt{1 - x \sin^2 \theta} \, d\theta$.

[34] See, e.g.,
      Landau L D and Lifshitz E M 1959 *Theory of Elasticity* (Reading, MA: Addison-Wesley)

[35] In some references, the deformation potential Ξ_{ij} is called the deformation potential tensor. In this paper, we refer to it just as a deformation potential.