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Linear response of a magnetized electron gas: application to the thermodynamics of aluminium

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Abstract. We first consider the three independent functions that describe the linear response to external perturbations of a *non-interacting* strongly magnetized electron gas. These functions are needed to build the *interacting* response to an external perturbation, even if it is purely scalar. The interacting response function is obtained in the local density approximation for the exchange and correlation energy functional $E^1_{xc}(n,\omega)$. It is singular when the non-interacting Fermi level coincides with a Landau band edge. In addition, the numerical study of the effective local-field factor shows that the response function can also have poles in a region of densities and magnetic fields approximately defined by: $r_s > 3.5$ and $0.3 \geqslant B/B_0 \geqslant 0.1$, where B_0 is the reference magnetic field (1 atomic unit $= 2.35 \times 10^9$ Gauss). Outside this region, we use the linear response theory applied to a model electron–ion interaction for an estimate of the equation of state of solid aluminium in the presence of strong magnetic fields up to $B = B_0$. The densities are in the range 0.8–1.5 times the normal density. The results show the importance of the changes induced by the magnetic field, in particular those associated with the localization of the charge density.

1. Introduction

The study of the structure of electronic systems in the presence of strong magnetic fields is a fast-developing area of atomic and solid-state physics. Its applications are no longer limited to astrophysics [1]. As the output of magnetic-field generators is increasing rapidly and is now reaching the range of 100 Tesla for non-destructive devices, many experiments are planned in several areas of condensed-matter physics [2]. If explosively driven implosion devices are considered, fields as high as 1400 Tesla are presently obtained [3]. These field values are those for which the electronic structure starts being affected in a non-trivial way [4]. From the theoretical point of view, the interplay between electron–electron interaction and magnetic effects is a very challenging problem. For this reason much study of free atoms in strong magnetic fields is presently being carried out. After the statistical approaches initiated in the seventies [5–15], the full self-consistent field problem is now being addressed. Hydrogen [16–34] and helium [16, 24, 35, 36] have been treated first, for instance in the Hartree–Fock (HF) approximation. More complex systems have been investigated [37], including H^- in excited states [38], molecules [39–42] and even atomic chains [43, 44]. Few heavier atoms, such as Li [45], C [43, 45] and Fe [43], have been calculated. In condensed matter, attention has been paid first to two-dimensional (2D) systems, in the context of the quantum hall effect [46] and for application to nanostructure design [47, 48]. Now three-dimensional (3D) systems are being investigated actively and this interest will increase in

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relation with the 'Dirac campaign' [2]. Another potential application of 3D studies concerns the Z-pinches experiments [49]. The numerical simulation of these experiments requires data on the equation of state and electrical conductivity, taking into account the effect of the magnetic field. The theoretical approach of condensed matter in the presence of strong fields is far more complex than the already difficult study of localized systems. The well established framework of HF theory is no use in these systems. The density functional theory (DFT), very popular in electronic structure calculations of condensed matter, has been extended to the magnetic case [50]. In the current-DFT (CDFT), the paramagnetic current becomes a second fundamental quantity [51]. But so far, the intensive numerical calculations that are necessary to give strong support to this theory are still lacking.

In this paper, we deal with the use of CDFT in simple delocalized condensed-matter systems. Our aim is to treat the effect of a weak scalar potential perturbation in a strongly magnetized electron gas (SMEG). The linear response theory of the SMEG is first reviewed. Because the exchange and correlation effects contribute not only to the scalar potential, but also to the vector potential, three response functions are involved. In section 2, we replace the linear-response theory in the context of the CDFT, recall results already published for two of the non-interacting response functions and give the expression of a third which gives the relation of the induced current with the perturbing vector potential. The local approximation of these response functions is also discussed. The limiting forms of the full response for long and short wavelengths are given in section 3. Section 4 deals with including exchange and correlation effects in the response functions, thus defining the effective local-field factor. Section 5 is devoted to numerical applications. First, the local-field factor is computed numerically, in a rather large domain of densities and magnetic-field intensities, and it is shown that it can induce singularities in the interacting response function. Second, the equation of state of metallic aluminium in the presence of strong magnetic fields is calculated and discussed.

2. Current density functional theory and linear response functions

2.1. General theory

The CDFT of Vignale and Rasolt [51] is a very convenient starting point for the analysis of the response of a SMEG to external perturbations. Although the linear response functions of the SMEG can be defined in standard second-order perturbation theory, we find it easier to introduce the local-field corrections (LFC) in the framework of CDFT. As will be seen later in this paper, a very compact expression of the LFC is obtained using the CDFT formalism.

The most important result of the CDFT is that the total energy of an electronic system, in the presence of an external scalar potential $V_{\rm ext}(\boldsymbol{r})$ and an external vector potential $\boldsymbol{A}(\boldsymbol{r})$, can be written:

$$E[n(\boldsymbol{r}),\boldsymbol{j}_p(\boldsymbol{r})] = T_s[n(\boldsymbol{r}),\boldsymbol{j}_p(\boldsymbol{r})] + E_H[n(\boldsymbol{r})] + \int n(\boldsymbol{r})\left[V_{\rm ext}(\boldsymbol{r}) + \frac{e^2}{2m}\boldsymbol{A}^2(\boldsymbol{r})\right]\mathrm{d}^3r$$
$$+e\int \boldsymbol{j}_p(\boldsymbol{r})\cdot\boldsymbol{A}(\boldsymbol{r})\,\mathrm{d}^3r + E_{\rm xc}[n(\boldsymbol{r}),\boldsymbol{j}_p(\boldsymbol{r})]. \qquad (2.1)$$

In this expression, e is the electron charge, m its mass, T_s is the noninteracting 'pseudo' kinetic energy (corresponding to the sum of the operators $-\hbar^2/2m\nabla^2$), E_H is the Coulomb electron–electron interaction energy and $E_{\rm xc}$ the exchange and correlation (xc) energy. The charge density is $n(\boldsymbol{r})$, and $\boldsymbol{j}_p(\boldsymbol{r})$ is the paramagnetic (orbital) current. The applied magnetic field is $\boldsymbol{B} = \nabla\wedge\boldsymbol{A}$. In this work, we neglect for simplicity the Landé magnetic moment

factor g which could be taken into account without special difficulty. The physical total current $\boldsymbol{J}$ is:

$$\boldsymbol{J}(\boldsymbol{r}) = \boldsymbol{j}_p(\boldsymbol{r}) + \frac{e}{m} n(\boldsymbol{r})\boldsymbol{A}(\boldsymbol{r}). \tag{2.2}$$

It is useful to introduce the new variable:

$$\boldsymbol{u}(\boldsymbol{r}) = \frac{\boldsymbol{j}_p(\boldsymbol{r})}{n(\boldsymbol{r})} \tag{2.3}$$

$n(\boldsymbol{r})$ and $\boldsymbol{u}(\boldsymbol{r})$ are independent quantities. A second result of the theory is to show that, for gauge invariance constraints, $E_{\rm xc}$ depends on $\boldsymbol{u}(\boldsymbol{r})$ through the variable $\nabla \wedge \boldsymbol{u}(\boldsymbol{r})$ only. This will be exploited in the treatment of xc effects.

The Euler–Kohn–Sham equations of the CDFT are obtained in writing the stationarity condition of the total energy for variations of $n(\boldsymbol{r})$ and $\boldsymbol{u}(\boldsymbol{r})$. They have been already discussed at length in the original work [51] and are not reproduced here.

Now we consider the case of a uniform system with density n, in the absence of an external scalar potential ($V_{\rm ext} = 0$). In this case, the physical current $\boldsymbol{J}$ vanishes, so that the paramagnetic current is: $\boldsymbol{j}_{\rm p0}(\boldsymbol{r}) = -\frac{e}{m} n\boldsymbol{A}(\boldsymbol{r})$, or $\boldsymbol{u}_0(\boldsymbol{r}) = -\frac{e}{m}\boldsymbol{A}(\boldsymbol{r})$. A weak scalar perturbing potential $\delta V_{\rm ext}(\boldsymbol{r})$ is then applied. It induces a charge density $\delta n(\boldsymbol{r})$ which screens the perturbation so that the total scalar potential becomes $\delta V(\boldsymbol{r})$ (δV does not include xc). Simultaneously, the vector potential is also perturbed and becomes $\boldsymbol{A}(\boldsymbol{r}) + \delta\boldsymbol{A}(\boldsymbol{r})$. The linear changes δn and $\delta\boldsymbol{u}$, are obtained by linearizing the Euler equations:

$$(S_s + S_{\rm xc})\delta n + (\boldsymbol{U}_s + \boldsymbol{U}_{\rm xc})^t \delta\boldsymbol{u} + \delta V = 0 \tag{2.4}$$

$$(\boldsymbol{U}_s + \boldsymbol{U}_{\rm xc})^* \delta n + ([\mathbf{M}_s] + [\mathbf{M}_{\rm xc}])\delta\boldsymbol{u} + en\delta\boldsymbol{A} = 0 \tag{2.5}$$

where the following notations have been used:

$$S_s = \left.\frac{\delta^2 T_s[n(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r})]}{\delta n(\boldsymbol{r})\delta n(\boldsymbol{r}')}\right|_0 \qquad S_{\rm xc} = \left.\frac{\delta^2 E_{\rm xc}[n(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r})]}{\delta n(\boldsymbol{r})\delta n(\boldsymbol{r}')}\right|_0 \tag{2.6}$$

$$\boldsymbol{U}_s = \left.\frac{\delta^2 T_s[n(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r})]}{\delta\boldsymbol{u}(\boldsymbol{r})\delta n(\boldsymbol{r}')}\right|_0 + e\boldsymbol{A}(\boldsymbol{r})\delta(\boldsymbol{r} - \boldsymbol{r}') \qquad \boldsymbol{U}_{\rm xc} = \left.\frac{\delta^2 E_{\rm xc}[n(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r})]}{\delta\boldsymbol{u}(\boldsymbol{r})\delta n(\boldsymbol{r}')}\right|_0 \tag{2.7}$$

$$[\mathbf{M}_s] = \left.\frac{\delta^2 T_s[n(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r})]}{\delta\boldsymbol{u}(\boldsymbol{r})\delta\boldsymbol{u}(\boldsymbol{r}')}\right|_0 \qquad [\mathbf{M}_{\rm xc}] = \left.\frac{\delta^2 E_{\rm xc}[n(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r})]}{\delta\boldsymbol{u}(\boldsymbol{r})\delta\boldsymbol{u}(\boldsymbol{r}')}\right|_0. \tag{2.8}$$

Equations (2.4) and (2.5) contain implicit convolution products in real space. The superscript t indicates transposition and $*$ the complex conjugate. In the following, we will use the superscript $+$ for the composed operation $t*$ (adjoint). The internal product $\boldsymbol{u} \cdot \boldsymbol{v}$ is thus also $\boldsymbol{u}^t\boldsymbol{v}$. In the following derivations, we use matrix notation preferably to tensor notation.

We note that the perturbation $\delta\boldsymbol{A}$ does not appear in the first equation. Notation $|_0$ means that the derivatives are taken for the uniform reference system. The Hamiltonian for this system contains the vector potential $\boldsymbol{A}(\boldsymbol{r})$ that is not translationally invariant. But a change of coordinates is equivalent to a gauge change. Therefore, any functional $F(\boldsymbol{r}, \boldsymbol{r}')$ associated with a physical quantity of the SMEG that is invariant in a gauge change is invariant in a translation. Its Fourier transform depends on one $\boldsymbol{q}$ vector only. This is the case, in particular, for the response functions of the magnetized electron gas, which expresses the density δn and the current $\delta\boldsymbol{J}$ in terms of the perturbations δV and $\delta\boldsymbol{A}$.

2.2. Non-interacting case

Let us first consider the non-interacting case, $E_{\rm xc} = 0$. The response functions are obtained in reciprocal space, with the help of equations (2.4) and (2.5).

The density/scalar potential response χ_{nV} (scalar) is:

$$\frac{1}{\chi_{nV}} = -S_s + \boldsymbol{U}_s^t[\mathbf{M}_s]^{-1}\boldsymbol{U}_s^*. \tag{2.9}$$

The current/scalar potential response $\chi_{\boldsymbol{J}V}$ (vector) is:

$$\chi_{\boldsymbol{J}V} = -n\chi_{nV}[\mathbf{M}_s]^{-1}\boldsymbol{U}_s^*. \tag{2.10}$$

The current/vector potential response $[\chi_{\boldsymbol{J}\boldsymbol{A}}]$ (matrix) is:

$$[\chi_{\boldsymbol{J}\boldsymbol{A}}] = e\frac{1}{\chi_{nV}}[\chi_{\boldsymbol{J}V}^*\chi_{\boldsymbol{J}V}^t] - \frac{en}{m}(mn[\mathbf{M}_s]^{-1} - [\mathbf{I}]). \tag{2.11}$$

Equations (2.9)–(2.11) show that the simultaneous knowledge of χ_{nV}, $\chi_{\boldsymbol{J}V}$ and $[\chi_{\boldsymbol{J}\boldsymbol{A}}]$ makes it possible to determine S_s, $\boldsymbol{U}_s$ and $[\mathbf{M}_s]^{-1}$. Therefore, the functional T_s to the second order in δn and $\delta\boldsymbol{u}$ is entirely determined by these three response functions. The energy expression involves $[\mathbf{M}_s]$: this means that, in practice, one must invert the matrix $[\mathbf{M}_s]^{-1}$ obtained from equation (2.11). The inversion can be performed analytically because the structure of $\chi_{\boldsymbol{J}V}$ and $[\chi_{\boldsymbol{J}\boldsymbol{A}}]$ is very special, as will be seen below.

Finally, the density/vector potential response function $\chi_{n\boldsymbol{A}}$ can be expressed in terms of the previous ones and is thus redundant.

2.3. Structure of the response functions

The response functions have been calculated using standard second-order perturbation theory for non-degenerate states. In particular, χ_{nV} has been extensively studied in the literature [53–56] and the numerical problems related to its computation are known [57]. We summarize here a few basic results in order to define notations that will be used in the following paragraphs.

The magnetic length λ is the important length scale in physical space. It is defined as:

$$\lambda^2 = \frac{\hbar}{m\omega} \tag{2.12}$$

and depends on the cyclotron frequency $\omega = eB/m$. The reduced matrix elements needed in all the response functions are:

$$k_{MN}(s) = \left(\frac{s}{\sqrt{2}}\right)^{M-N}\sqrt{\frac{N!}{M!}}\exp\left(-\frac{1}{4}s^2\right)L_N^{M-N}\left(\frac{1}{2}s^2\right) \tag{2.13}$$

where $N(M)$ is a Landau band index. Equation (2.13) is valid if $N \leqslant M$ and must be supplemented with:

$$k_{MN}(s) = (-1)^{M-N}k_{NM}(s)$$

when $M < N$. In the previous formulae, $L_N^Q(x)$ is the Laguerre polynomial defined in [58]. Two other functions must also be introduced. They are:

$$\mathrm{G}_{MN}(t) = \frac{1}{t}\ln\left|\frac{(t-y_N)^2 - y_M^2}{(t+y_N)^2 - y_M^2}\right| \tag{2.14}$$

$$\mathrm{H}_{MN}(t) = \frac{1}{t^2}[-2y_N + (N-M)\mathrm{G}_{MN}(t)] \tag{2.15}$$

with:

$$y_N^2 = 2\left(\frac{\mu}{\hbar\omega} - \left(N + \frac{1}{2}\right)\right) \tag{2.16}$$

where μ is the non-interacting Fermi energy. The uniform density of the unperturbed system can be expressed in terms of the quantities y_N:

$$n = \frac{1}{\pi^2\lambda^3}\sum_N f_N y_N \tag{2.17}$$

where $f_N = 1$ if the Landau band of index N contains electrons and 0 if it is empty (in the latter case, y_N would be imaginary). Let us give the expressions of the response functions.

2.3.1. The density/scalar potential response function. The function can be written [52, 59]:

$$\chi_{nV} = \frac{1}{\pi^2\lambda^3\overline{h}\omega}K(q_\perp\lambda, q_z\lambda) \tag{2.18a}$$

where q_z and $q_\perp$ are the components of $\boldsymbol{q}$ parallel and perpendicular to $\boldsymbol{B}$ respectively, and:

$$K(s,t) = \sum_M\sum_N f_N k_{MN}(s)k_{MN}(s)\mathrm{G}_{MN}(t). \tag{2.18b}$$

From the definition of $\mathrm{G}_{MN}(t)$, one sees that this response function has singularities for the values of $t = q_z\lambda$ such that:

$$t = \pm y_N \pm y_M \qquad \text{and} \qquad t = \pm y_N \mp y_M$$

provided that y_M is real, i.e. for $M \leqslant N$. The integral of $\mathrm{G}_{MN}(t)$ in the vicinity of the singularities is convergent.

2.3.2. Current/scalar potential response vector. This has already been studied by Skudlarski and Vignale [52]. Here we write it in a different, but rigorously equivalent, form:

$$\chi_{\boldsymbol{J}V} = \frac{\overline{h}}{m\lambda}\chi_{nV}X(q_\perp\lambda, q_z\lambda)\mathrm{i}\frac{\boldsymbol{q}}{q_\perp}\wedge\boldsymbol{e}_z \tag{2.19a}$$

with:

$$X(s,t) = \frac{1}{K(s,t)}\sum_M\sum_N f_N k_{MN}(s)p_{MN}(s)\mathrm{G}_{MN}(t) \tag{2.19b}$$

$$p_{MN}(s) = \sqrt{\frac{N+1}{2}}k_{M,N+1}(s) - \sqrt{\frac{N}{2}}k_{M,N-1}(s) \tag{2.19c}$$

It can be checked that $\boldsymbol{q}\cdot\delta\boldsymbol{J}(\boldsymbol{q}) = \boldsymbol{q}\cdot\chi_{\boldsymbol{J}V}(\boldsymbol{q})\delta V(q) = 0$, a necessary requirement for the conservation of the physical current.

2.3.3. Current/vector potential response matrix. Obtaining the expression to this matrix is slightly more complicated. To our knowledge it has not been published so far, at least in a form similar to the previous two response functions. This expression is:

$$[\chi_{\boldsymbol{J}\boldsymbol{A}}] = e\left(\frac{\overline{h}}{m\lambda}\right)^2\chi_{nV}[Y(q_\perp\lambda, q_z\lambda)[\mathbf{O}_2] + Z(q_\perp\lambda, q_z\lambda)[\mathbf{P}_3]] \tag{2.20a}$$

where the matrices $[\mathbf{O}_2]$ and $[\mathbf{P}_3]$ are:

$$[\mathbf{O}_2] = \begin{vmatrix} \left(\frac{q_y}{q_\perp}\right)^2 & -\frac{q_y q_x}{q_\perp^2} & 0 \\ -\frac{q_x q_y}{q_\perp^2} & \left(\frac{q_x}{q_\perp}\right)^2 & 0 \\ 0 & 0 & 0 \end{vmatrix}$$
$$[\mathbf{P}_3] = \begin{vmatrix} \left(\frac{q_z}{q}\right)^2 & 0 & -\frac{q_z q_x}{q^2} \\ 0 & \left(\frac{q_z}{q}\right)^2 & -\frac{q_z q_y}{q^2} \\ -\frac{q_x q_z}{q^2} & -\frac{q_y q_z}{q^2} & \left(\frac{q_\perp}{q}\right)^2 \end{vmatrix}. \tag{2.20b}$$

The functions Y and Z are defined as:

$$Y(s,t) = \frac{1}{K(s,t)} \sum_M \sum_N f_N [p_{MN}(s) - t_{MN}(s)][p_{MN}(s) + t_{MN}(s)] \mathrm{G}_{MN}(t) \tag{2.20c}$$

$$Z(s,t) = -\frac{1}{K(s,t)} \sum_M \sum_N f_N \frac{s^2 + t^2}{s} k_{MN}(s) t_{MN}(s) \mathrm{H}_{MN}(t) \tag{2.20d}$$

$$t_{MN}(s) = \sqrt{\frac{N+1}{2}} k_{M,N+1}(s) + \sqrt{\frac{N}{2}} k_{M,N-1}(s) + \frac{1}{2} s k_{MN}(s). \tag{2.20e}$$

The condition for conservation of the physical current $\boldsymbol{q} \cdot [\chi_{\boldsymbol{JA}}] \delta \boldsymbol{A}(\boldsymbol{q}) = 0$ is fulfilled. In addition, $\delta \boldsymbol{J}$ is gauge invariant: if $\delta \boldsymbol{A}$ is changed to $\delta \boldsymbol{A} + \nabla \Lambda$, with Λ an arbitrary function, any of the components of $\delta \boldsymbol{J}$ vanishes.

For obtaining an explicit form of $[\mathbf{M}_s]$ that can be used directly in the calculation of the kinetic energy, one starts from equation (2.11) which, with the help of equations (2.19*a*) and (2.20*a*), can be written:

$$mn[\mathbf{M}_s]^{-1} = [\mathbf{I}] + C[(-X^2 + Y)[\mathbf{O}_2] + Z[\mathbf{P}_3]] \tag{2.21}$$

with:

$$C = -\frac{m}{n} \left(\frac{\overline{h}}{m\lambda}\right)^2 \chi_{nV}. \tag{2.22}$$

In the previous equations, the dependence of χ_{nV}, X, Y and Z on $q_\perp \lambda$ and $q_z \lambda$ has been omitted for the sake of simplicity. Now we introduce the matrix $[\mathbf{O}_3]$:

$$[\mathbf{O}_3] = \begin{vmatrix} 1 - \left(\frac{q_x}{q}\right)^2 & -\frac{q_y q_x}{q^2} & -\frac{q_z q_x}{q^2} \\ -\frac{q_x q_y}{q^2} & 1 - \left(\frac{q_y}{q}\right)^2 & -\frac{q_z q_y}{q^2} \\ -\frac{q_x q_z}{q^2} & -\frac{q_y q_z}{q^2} & 1 - \left(\frac{q_z}{q}\right)^2 \end{vmatrix} \tag{2.23a}$$

that fulfils the relations:

$$q^2[\mathbf{O}_3] - q^2[\mathbf{P}_3] - q_\perp^2[\mathbf{O}_2] = 0 \tag{2.23b}$$

where $[\mathbf{O}_2]$ and $[\mathbf{P}_3]$ are defined by equation (2.20*b*). $[\mathbf{O}_2]$ and $[\mathbf{O}_3]$ are nilpotent and their product satisfies:

$$[\mathbf{O}_3][\mathbf{O}_2] = [\mathbf{O}_2][\mathbf{O}_3] = [\mathbf{O}_2]. \tag{2.24}$$

Using equations (2.23) and (2.24), equation (2.21) can be inverted to give:

$$\frac{1}{mn}[\mathbf{M}_s] = [\mathbf{I}] + \frac{1}{1 + CZ} \frac{C(X^2 - Y + Z(q_\perp/q)^2)}{1 + CZ - C(X^2 - Y + Z(q_\perp/q)^2)} [\mathbf{O}_2] - \frac{CZ}{1 + CZ} [\mathbf{O}_3]. \tag{2.25}$$

2.4. Local approximation of the kinetic energy

After Landau's work [60], the solutions of the Schrödinger equation for a free electron in a magnetic field are well known. From the eigenvalues, one deduces the explicit expression of the energy density for the uniform non-interacting electron gas in a magnetic field:

$$e_s(n,\omega) = \frac{1}{2\pi^2\lambda^3}\overline{h}\omega\left(\frac{1}{3}\boldsymbol{S}_{30} + 2\boldsymbol{S}_{11}\right) \tag{2.26}$$

where use has been made of the simplifying notations:

$$\boldsymbol{S}_{pq} = \sum_N f_N (y_N)^p (N+\tfrac{1}{2})^q \tag{2.27}$$

with y_N defined in equation (2.16). The kinetic component of the total energy associated with equation (2.26) is given by:

$$T_s[n, \boldsymbol{u_0}(\boldsymbol{r})] = \int e_s(n,\omega)\,\mathrm{d}^3r + \frac{m}{2}\int n\boldsymbol{u}_{\boldsymbol{0}}^2(\boldsymbol{r})\,\mathrm{d}^3r. \tag{2.28}$$

In a homogeneous system, the local approximation amounts to using this expression with the local values of the density and the current defined in every point $\boldsymbol{r}$. In this local approximation, the kinetic energy is thus:

$$T_s^1[n(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r})] = \int e_s(n(\boldsymbol{r}), \omega(\boldsymbol{r}))\,\mathrm{d}^3r + \frac{m}{2}\int n(\boldsymbol{r})\boldsymbol{u}^2(\boldsymbol{r})\,\mathrm{d}^3r \tag{2.29}$$

with $\omega(\boldsymbol{r})$ defined by:

$$\omega(\boldsymbol{r}) = |\nabla \times \boldsymbol{u}(\boldsymbol{r})|. \tag{2.30}$$

In the uniform case, $\omega = |\nabla \times \boldsymbol{u}_0(\boldsymbol{r})| = \frac{eB}{m}$. It is possible, in the local approximation, to calculate explicitly all the derivatives defined in equations (2.6)–(2.8). In the following, all the derivatives are taken with respect to the two independent variables n and ω. For the partial derivatives, the variable held fixed is not indicated. One finds:

$$S_s^1 = \frac{\partial^2 e_s(n,\omega)}{\partial n^2} = \frac{\partial \mu}{\partial n} \tag{2.31a}$$

$$\frac{\partial^2 e_s(n,\omega)}{\partial n^2} = \pi^2\lambda^3\overline{h}\omega\frac{1}{\boldsymbol{S}_{-10}}. \tag{2.31b}$$

The vector $\boldsymbol{U}_s^1$ is, in reciprocal space:

$$\boldsymbol{U}_s^1 = -\frac{\partial^2 e_s(n,\omega)}{\partial n\partial\omega}\mathrm{i}\boldsymbol{q}\wedge\boldsymbol{e}_z \tag{2.32a}$$

$$\frac{\partial^2 e_s(n,\omega)}{\partial n\partial\omega} = \overline{h}\frac{\boldsymbol{S}_{-11} - \boldsymbol{S}_{10}}{\boldsymbol{S}_{-10}}. \tag{2.32b}$$

The matrix $[\mathbf{M}_s^1]$ involves first and second derivatives with respect to ω:

$$[\mathbf{M}_s^1] = mn[\mathbf{I}] + \left(\frac{\partial^2 e_s(n,\omega)}{\partial\omega^2} - \frac{1}{\omega}\frac{\partial e_s(n,\omega)}{\partial\omega}\right)q_\perp^2[\mathbf{O}_2] + \frac{1}{\omega}\left(\frac{\partial e_s(n,\omega)}{\partial\omega}\right)q^2[\mathbf{O}_3]. \tag{2.33}$$

Using equation (2.26), one gets:

$$\frac{\partial e_s(n,\omega)}{\partial\omega} = \frac{\overline{h}}{\pi^2\lambda^3}\left(\boldsymbol{S}_{11} - \frac{1}{3}\boldsymbol{S}_{31}\right) \tag{2.34a}$$

$$\frac{\partial^2 e_s(n,\omega)}{\partial\omega^2} = \frac{\overline{h}}{\pi^2\lambda^3}\frac{1}{\omega}\left[\frac{(\boldsymbol{S}_{-11} - \boldsymbol{S}_{10})^2}{\boldsymbol{S}_{-10}} + (2\boldsymbol{S}_{11} - \boldsymbol{S}_{-12})\right]. \tag{2.34b}$$

Inverting equation (2.33) with the help of equations (2.21) and (2.25), one obtains:

$$[\mathbf{M}_s^1]^{-1}\boldsymbol{U}_s^{1*} = \mathrm{i}\boldsymbol{q}\wedge\boldsymbol{e}_z\frac{\partial\mu}{\partial\omega}\left[mn+\frac{\partial^2 e_s(n,\omega)}{\partial\omega^2}q_\perp^2+\frac{1}{\omega}\frac{\partial e_s(n,\omega)}{\partial\omega}q_z^2\right]^{-1} \tag{2.35}$$

and, with the definition in equation (2.9):

$$\frac{1}{\chi_{nV}^1} = -\left(\frac{\partial\mu}{\partial n}\right)_\omega + q_\perp^2\left(\frac{\partial\mu}{\partial\omega}\right)^2\left[mn+\frac{\partial^2 e_s(n,\omega)}{\partial\omega^2}q_\perp^2+\frac{1}{\omega}\frac{\partial e_s(n,\omega)}{\partial\omega}q_z^2\right]^{-1}. \tag{2.36}$$

Equations (2.35) and (2.36), together with equation (2.10), lead straightforwardly to the expression of $\chi_{\boldsymbol{J}V}^1$. All the expressions shown above are more than low-order expansions, they are exact expressions in the framework of the local-density approximation.

3. Response functions in limiting cases

The behaviour of the response functions in the limits of small and large q is the basis for defining approximate kinetic-energy functionals. We present in this section some results for these limits and, as an example, derive a functional generalizing the gradient expansion, well known in the absence of a magnetic field.

3.1. Small q limit

Starting with the expansion of $k_{MN}(s)$, equation (2.13), for small s and using the expansion of the functions $\mathrm{G}_{MN}(t)$ and $\mathrm{H}_{MN}(t)$, equations (2.14) and (2.15), for small t, one obtains the behaviour of the response functions for $q_\perp$ and q_z going to zero.

The limit of $\chi_{nV}(\boldsymbol{q})$ is:

$$\chi_{nV}(\mathbf{0}) = -\frac{1}{\pi^2\lambda^3\hbar\omega}\boldsymbol{S}_{-10} = -\left(\frac{\partial n}{\partial\mu}\right)_\omega. \tag{3.1}$$

Comparing with equation (2.36), one sees that:

$$\chi_{nV}(\mathbf{0}) = \chi_{nV}^1(\mathbf{0}). \tag{3.2}$$

To first order in q^2, one obtains:

$$\chi_{nV}(\boldsymbol{q}) = \chi_{nV}(\mathbf{0}) + \frac{1}{\pi^2\lambda\hbar\omega}\left(q_\perp^2(\boldsymbol{S}_{-11}-\boldsymbol{S}_{10}) - \frac{1}{12}q_z^2\boldsymbol{S}_{-30}\right). \tag{3.3}$$

Equation (3.1) contains the sum $\boldsymbol{S}_{-10}$ of the inverses of the quantities y_N. If it happens that the non-interacting Fermi energy μ is located just on the edge of the Landau band of index N_m, (i.e. $y_{N_m} = 0$), then the response function $\chi_{nV}(\mathbf{0})$ goes to infinity. This means that, under these particular conditions, the wavefunction for the system perturbed by δV cannot be constructed as an expansion in unperturbed wavefunctions. Although the degeneracy of electron states in the x, y-plane is removed by the electronic motion in the z-direction (parallel to the magnetic field), the number of states per unit energy near the Fermi level, which is proportional to $1/y_{N_m}$, becomes infinite and causes the divergence of the perturbation series.

For $\chi_{\boldsymbol{J}V}$, the small q behaviour, as deduced from equation (2.19*a*), is:

$$\chi_{\boldsymbol{J}V} = \frac{\hbar}{m\lambda}\frac{1}{\pi^2\lambda^3\hbar\omega}(\boldsymbol{S}_{-11}-\boldsymbol{S}_{10})(q_\perp\lambda)\mathrm{i}\frac{\boldsymbol{q}}{q_\perp}\wedge\boldsymbol{e}_z \tag{3.4a}$$

$$= -\frac{1}{m}\left(\frac{\partial\mu}{\partial\omega}\right)_n\chi_{nV}(\mathbf{0})\mathrm{i}\boldsymbol{q}\wedge\boldsymbol{e}_z \tag{3.4b}$$

which shows that, to the lowest order in q:

$$\chi_{JV} = \chi^1_{JV}. \tag{3.5}$$

We also deduce the limiting form of the function $X(s,t)$, equation (2.19*b*):

$$\frac{X(s,t)}{s} = -\frac{1}{\bar{h}}\left(\frac{\partial\mu}{\partial\omega}\right)_n = -\frac{1}{\boldsymbol{S}_{-10}}(\boldsymbol{S}_{-11} - \boldsymbol{S}_{10}). \tag{3.6}$$

The study of the functions appearing in $[\chi_{JA}]$ indicates that, for small q:

$$\frac{Y(s,t)}{s^2} = -\frac{1}{\boldsymbol{S}_{-10}}(2\boldsymbol{S}_{11} - \boldsymbol{S}_{-12}) \tag{3.7}$$

$$\frac{Z(s,t)}{s^2+t^2} = \frac{1}{\boldsymbol{S}_{-10}}\left(\frac{1}{3}\boldsymbol{S}_{30} - \boldsymbol{S}_{11}\right). \tag{3.8}$$

Going back to equation (2.25), one finds the expression of $[\mathbf{M}_s]$ to the order q^2 inclusively:

$$\frac{1}{mn}[\mathbf{M}_s] = [\mathbf{I}] + C(X^2 - Y)[\mathbf{O}_2] - CZ[\mathbf{P}_3]. \tag{3.9}$$

Using equations (3.6)–(3.9), one establishes that the low q limit of $[\mathbf{M}_s]$ is identical to the expression of its counterpart calculated in the local approximation, as given in equation (2.33):

$$[\mathbf{M}_s] = [\mathbf{M}^1_s].$$

Thus the important result of this paragraph is that, *to the lowest order in q*, the three quantities S_s, $\boldsymbol{U}_s$ and $[\mathbf{M}^1_s] - mn[\mathbf{I}]$, defined in chapter 2 in terms of the exact functional $T_s[n(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r})]$, are identical to the similar quantities obtained with the local functional $T^1_s[n(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r})]$. One can check that equation (3.3), which gives the expression for the response function $\chi_{nV}(\boldsymbol{q})$ for small $\boldsymbol{q}$ goes correctly to the corresponding expression, deduced from the Lindhard response function, when the magnetic field B vanishes.

3.2. Large q limit

The complete mathematical study of the large q behaviour of the response functions is rather complicated in the present formulation. This study is easier when done using the integral form of the response function [54]. However, instead of introducing the latter now (which is not well suited for numerical calculations) it would be easier to use a more direct procedure which takes advantage of analogies between the limits for large q and for the vanishing magnetic field.

The expressions of the response functions given in section 2 show that their dependence on $\boldsymbol{q}$ occurs always through the dimensionless variables $s = q_\perp\lambda$ and $t = q_z\lambda$ (λ is proportional to $\sqrt{B}$). The asymptotic form for large $\boldsymbol{q}$ is thus related to the asymptotic form for B going to zero. In those cases where the limit for $B = 0$ is finite, it gives the behaviour for large $\boldsymbol{q}$. This analogy is helpful for χ_{nV} and χ_{JA} (or $[\mathbf{M}_s]$), but not for χ_{JV} which vanishes identically for $B = 0$. We illustrate these analogies in the following paragraph.

Let us consider first χ_{nV}. Expanding the magnetic response, equation (2.18*a*), for large $s = q_\perp\lambda$ and $t = q_z\lambda$ gives:

$$\chi_{nV}(\boldsymbol{q}) = -\frac{4m}{\bar{h}^2}\frac{n}{q_z^2}\left(1 - \frac{q_\perp^2}{q_z^2}\right) + \frac{1}{q_z^4}\gamma\omega^{5/2}\boldsymbol{S}_{30} \tag{3.10}$$

where γ is a coefficient which does not depend on ω. The next terms in the expansion are of order q_z^{-6}. In the limit $\omega \to 0$, it can be shown that:

$$\boldsymbol{S}_{30} = \frac{4\sqrt{2}}{5}\left(\frac{\mu}{\hbar\omega}\right)^{5/2} \tag{3.11}$$

so that, in this limit:

$$\chi_{nV}(\boldsymbol{q}) = -\frac{4m}{\hbar^2}\frac{n}{q_z^2}\left[\left(1 - \frac{q_\perp^2}{q_z^2}\right) + \frac{4k_F^2}{5q_z^2} + \cdots\right]. \tag{3.12}$$

To order q_z^{-4}, this last expansion is equivalent to the Lindhard function $\chi_L(q)$, the well known response at $B = 0$. When the field B is finite, one can write, for large q:

$$\chi_{nV}(\boldsymbol{q}) \to -\frac{4m}{\hbar^2}\frac{n}{q^2} + \frac{1}{q^4}\delta\left(\omega, \frac{q_\perp^2}{q^2}\right) \tag{3.13}$$

where δ is a function whose more precise definition is useless here.

The response function χ_{JV} is identically zero for $B = 0$ because a scalar potential does not induce currents in the non-magnetized case. The expansion that can be derived starting from equation (2.19*a*) must be consistent with this limit. Expanding for large q, the leading term is found to be:

$$\chi_{JV}(\boldsymbol{q}) = \frac{4m}{\hbar^2}\omega n\frac{1}{q^3}\mathrm{i}\frac{\boldsymbol{q}}{q} \wedge \boldsymbol{e}_z \tag{3.14}$$

which vanishes for $B = 0$, as expected.

We come now to the behaviour of $[\mathbf{M}_s]$ for large $\boldsymbol{q}$. In the limit $B = 0$, the current/vector potential response function is known [61]:

$$mn[\mathbf{M}_s]^{-1} = [\mathbf{I}] - F\left(\frac{q}{2k_F}\right)[\mathbf{O}_3] \tag{3.15a}$$

with:

$$F(y) = \frac{3}{8}(y^2+1) - \frac{3}{16}\frac{(1-y^2)^2}{y}\ln\left|\frac{1+y}{1-y}\right|. \tag{3.15b}$$

The expansion of F for y infinite is: $1 - \frac{1}{5}y^{-2}$. We will show that this limit can be found from the general expression of $[\mathbf{M}_s]$, equation (2.25). For large t, equations (2.19*b*), (2.20*c*) and (2.20*d*) give:

$$X(s,t) = -\frac{s}{s^2+t^2} \tag{3.16}$$

$$Y(s,t) = -\frac{s^2}{4} \tag{3.17}$$

$$Z(s,t) = -\frac{s^2+t^2}{4} \tag{3.18}$$

$$1 + CZ = \frac{4}{5}\frac{k_F^2}{q^2}. \tag{3.19}$$

With these expressions in equation (2.25):

$$\frac{1}{mn}[\mathbf{M}_s] = [\mathbf{I}] + 5\left(\frac{q}{2k_F}\right)^2[\mathbf{O}_3] \tag{3.20a}$$

or, to order q^{-2} inclusively:

$$mn[\mathbf{M}_s]^{-1} = [\mathbf{I}] - \left(1 - \frac{1}{5}y^{-2}\right)[\mathbf{O}_3] \tag{3.20b}$$

which agrees with the large $\boldsymbol{q}$ limit of equation (3.15*a*).

The results of this study of the response functions limits for small and large $\boldsymbol{q}$ can be applied to the definition of approximate kinetic-energy functionals which generalize the well known approximations for the zero field [62] to the case of finite magnetic fields. These approximate functionals are: (i) the gradient expansion functional and (ii) the Thomas–Fermi–Von Weizsäcker functional. As an illustration, we derive in the following section the gradient-expansion functional in the presence of a magnetic field.

3.3. Gradient expansion

In the absence of a magnetic field, this approximation consists in using as the kinetic-energy functional the local functional supplemented by a correction which, when linearized with respect to the density $\delta n(\boldsymbol{r})$, gives the correct term of order q^2 in the linear response. For zero field, the local functional is given by the Thomas–Fermi approximation $e_s(n(\boldsymbol{r}), 0)$:

$$e_s(n(\boldsymbol{r}), 0) = \frac{3}{10}(3\pi^2)^{2/3}\frac{\overline{h}^2}{m}(n(\boldsymbol{r}))^{5/3} \tag{3.21}$$

and the correction is:

$$\delta e_s(n(\boldsymbol{r}), 0) = \frac{\overline{h}^2}{72m}\frac{|\nabla n(\boldsymbol{r})|^2}{n(\boldsymbol{r})}. \tag{3.22}$$

When a magnetic field is applied, the local functional gives the exact behaviour of S_s to the order q^0, of $\boldsymbol{U}_s$ to the order q^1 (the term in q^2 does not exist) and of $[\mathbf{M}_s]$ to the order q^2. Therefore, the only additional correction required to have the exact expansion of the full functional to the order q^2 comes from the q^2 term in S_s. The corresponding correction, derived from the response functions, is:

$$\delta e_s(n, \omega) = \tfrac{1}{2}\delta n(\boldsymbol{q})(S_s(\boldsymbol{q}) - S_s^1(\boldsymbol{q}))_2\delta n(\boldsymbol{q}) \tag{3.23}$$

where the subscript 2 means that only the terms of the order q^2 in the difference are kept. This correction is obtained from the difference of the inverses of the response functions χ_{nV}. Finally, in the gradient expansion approximation, the kinetic energy is:

$$T_s^{gr}[n(\boldsymbol{r}), \boldsymbol{u}(\boldsymbol{r})] = \int e_s(n(\boldsymbol{r}), \omega(\boldsymbol{r}))\,\mathrm{d}^3r + \frac{m}{2}\int n(\boldsymbol{r})\boldsymbol{u}^2(\boldsymbol{r})\,\mathrm{d}^3r + \int \delta e_s(n(\boldsymbol{r}), \omega(\boldsymbol{r}))\,\mathrm{d}^3r \tag{3.24a}$$

$$\delta e_s(n(\boldsymbol{r}), \omega(r)) = \frac{\overline{h}^2}{2m}\alpha(n(\boldsymbol{r}), \omega(\boldsymbol{r}))\frac{|\nabla_\perp n(\boldsymbol{r})|^2}{n(\boldsymbol{r})} - \frac{\overline{h}^2}{24m}\beta(n(\boldsymbol{r}), \omega(\boldsymbol{r}))\frac{|\nabla_z n(\boldsymbol{r})|^2}{n(\boldsymbol{r})} \tag{3.24b}$$

$$\alpha(n, \omega) = \frac{1}{(\boldsymbol{S}_{-10})^2}(\boldsymbol{S}_{-11} - \boldsymbol{S}_{10})\boldsymbol{S}_{11} \tag{3.25a}$$

$$\beta(n, \omega) = \frac{1}{(\boldsymbol{S}_{-10})^2}\boldsymbol{S}_{-30}\boldsymbol{S}_{10}. \tag{3.25b}$$

The functions α and β are calculated with the local values for n and ω. This functional is defined for any index of the highest populated Landau band. It is not restricted to the first band ($N = 0$), as is the case for the functional proposed by Tomishima and Shinjo [11]. Finally, even in the case $N = 0$, it does not reduce to the form given by these authors who also expanded $e_s(n(\boldsymbol{r}), \omega(\boldsymbol{r}))$ to the second order in $\nabla\omega(r)$.

In relation with the singularities of the sums $\boldsymbol{S}_{pq}$, for negative values of p, when the Fermi level coincides exactly with a band edge, use of the functional in equation (3.24) can lead to difficulties if there are points in space where these sums go locally to infinity. In

such cases, $\alpha(n(\boldsymbol{r}), \omega(\boldsymbol{r}))$ remains finite but $\beta(n(\boldsymbol{r}), \omega(\boldsymbol{r}))$ diverges like $1/y_{N_m}$, N_m being the index of the first empty band.

4. Effective local-field factor

We consider now an electron gas of average density n in the presence of a uniform magnetic field B, perturbed by an external scalar potential. The external vector potential is unperturbed. Such a system may be viewed as a model for an ion embedded in a magnetized electron gas. It can be treated by an extension to the magnetic case of the pseudo or model potential method commonly applied to the calculation of bulk properties of simple metals such as, for instance, their equation of state.

Equations (2.4) and (2.5) with $\delta \boldsymbol{A} = 0$ are the starting point of the method. Eliminating the current, one arrives at:

$$(S_s + S_{\rm xc})\delta n - (\boldsymbol{U}_s + \boldsymbol{U}^1_{\rm xc})^t([\mathbf{M}_s] + [\mathbf{M}^1_{\rm xc}])^{-1}(\boldsymbol{U}_s + \boldsymbol{U}^1_{\rm xc})^*\delta n + \delta V = 0. \tag{4.1}$$

Introducing the non-interacting response function given in equation (2.9), one can write:

$$\left(-\frac{1}{\chi_{nV}} + Q(\boldsymbol{q})\right)\delta n = -\delta V \tag{4.2}$$

with:

$$Q(\boldsymbol{q}) = Q_n(\boldsymbol{q}) + Q_u(\boldsymbol{q}) \tag{4.3a}$$

$$Q_n(\boldsymbol{q}) = S_{\rm xc}(\boldsymbol{q}) \tag{4.3b}$$

$$Q_u(\boldsymbol{q}) = \boldsymbol{U}_s^t[\mathbf{M}_s]^{-1}\boldsymbol{U}_s^* - (\boldsymbol{U}_s + \boldsymbol{U}^1_{\rm xc})^t([\mathbf{M}_s] + [\mathbf{M}^1_{\rm xc}])^{-1}(\boldsymbol{U}_s + \boldsymbol{U}^1_{\rm xc})^*. \tag{4.3c}$$

In the interacting case, the response function which relates the density δn to the external scalar potential $V_{\rm ext}$ is:

$$\tilde{\chi}_{nV}(\boldsymbol{q}) = \frac{\chi_{nV}(\boldsymbol{q})}{1 - \left(\frac{4\pi}{q^2} + Q(\boldsymbol{q})\right)\chi_{nV}(\boldsymbol{q})}. \tag{4.4}$$

$Q(\boldsymbol{q})$ is the effective local-field factor, entirely defined by the exchange and correlation energy functional $E_{\rm xc}[n(\boldsymbol{r}), u(\boldsymbol{r})]$. In the absence of a magnetic field, the component $Q_u(\boldsymbol{q})$ is zero. If a local approximation $E^1_{\rm xc}$ is used for $E_{\rm xc}$, $Q_n(\boldsymbol{q})$ is a constant, it does not depend on q and is simply given by the second derivative of $E^1_{\rm xc}$ with respect to the density, calculated for the uniform density n. If a non-local approximation is used, then Q_n depends explicitly on q.

The behaviour of the response function defined in equation (4.4), when χ_{nV} diverges because the non-interacting Fermi level coincides with a Landau band edge, is:

$$\tilde{\chi}_{nV}(\boldsymbol{q}) = -\frac{1}{\frac{4\pi}{q^2} + Q(\boldsymbol{q})}.$$

Since Q is negative, there exist values of the vector $\boldsymbol{q}$ for which $\tilde{\chi}_{nV}(\boldsymbol{q})$ is singular. The singularity stems from the fact that the interacting response function cannot be constructed, in these cases, from the non-interacting response function [52]. The correlations play a dominant role: they modify the Landau bands population and avoid the fact that any one can contain an infinitesimal number of electrons [59, 63].

In case the highest populated band contains a finite number of electrons, other mechanisms can induce poles in the interacting response function. They will be discussed in section 5.1.

For finite magnetic fields, little information is available on the electron-gas exchange and correlation energy. So far, the only known estimate has been published by Skudlarski and Vignale [59]. These authors have calculated the change $\Delta E^1_{\rm xc}(n,\omega) = E^1_{\rm xc}(n,\omega) - E^1_{\rm xc}(n,0)$ in the random phase approximation (RPA), in the non-polarized case ($g = 0$). This approximation is asymptotically exact at high density, when the density parameter $r_s(4\pi r_s^3 n/3 = 1)$ verifies:

$$r_s < \min\left(1; \left(\frac{\mu}{\hbar\omega} - \frac{1}{2}\right)^{1/3}\right).$$

Nevertheless, it is admitted that the RPA is a reasonable approximation at zero magnetic field, for larger values of r_s, in the metallic regime. To obtain the total exchange and correlation energy, one can add to $\Delta E^1_{\rm xc}(n,\omega)$ the $B = 0$ contribution $E^1_{\rm xc}(n,0)$ calculated in the most accurate approximation available. One must then use the local density approximation:

$$E^1_{\rm xc}(n(\boldsymbol{r}), u(\boldsymbol{r})) = \int e^1_{\rm xc}(n(\boldsymbol{r}), \omega(\boldsymbol{r}))\, {\rm d}^3 r. \tag{4.5}$$

We calculate now $Q(\boldsymbol{q})$ explicitly. From equations (2.10) and (2.19*a*), one obtains:

$$\boldsymbol{U}^*_s = -\frac{\overline{h}}{mn\lambda} X[\mathbf{M}_s] {\rm i}\frac{\boldsymbol{q}}{q_\perp} \wedge \boldsymbol{e}_z \tag{4.6}$$

where, for the sake of clarity, the arguments of the function $X(s,t)$ have been omitted. The local xc contribution can be calculated in analogy with the derivation of the local kinetic functional:

$$\boldsymbol{U}^{1*}_{\rm xc} = \frac{\partial^2 e^1_{\rm xc}}{\partial n \partial \omega} {\rm i}\boldsymbol{q} \wedge \boldsymbol{e}_z. \tag{4.7}$$

The matrix $[\mathbf{M}_s]$ is obtained starting from equation (2.25). It is written as:

$$[\mathbf{M}_s] = mn[\mathbf{I}] + R_s q_\perp^2 [\mathbf{O}_2] + W_s q^2 [\mathbf{O}_3] \tag{4.8}$$

and for $[\mathbf{M}^1_{\rm xc}]$, one applies the relations found in the local approximation (see equation (2.33)):

$$[\mathbf{M}^1_{\rm xc}] = R^1_{\rm xc} q_\perp^2 [\mathbf{O}_2] + W^1_{\rm xc} q^2 [\mathbf{O}_3] \tag{4.9}$$

with:

$$R^1_{\rm xc} = \frac{\partial^2 e^1_{\rm xc}}{\partial \omega^2} - \frac{1}{\omega}\frac{\partial e^1_{\rm xc}}{\partial \omega} \tag{4.10a}$$

$$W^1_{\rm xc} = \frac{1}{\omega}\frac{\partial e^1_{\rm xc}}{\partial \omega}. \tag{4.10b}$$

Adding these two matrices gives:

$$[\mathbf{M}_t] = [\mathbf{M}_s] + [\mathbf{M}^1_{\rm xc}] = mn[\mathbf{I}] + R_t q_\perp^2 [\mathbf{O}_2] + W_t q^2 [\mathbf{O}_3] \tag{4.11}$$

with $R_t = R_s + R^1_{\rm xc}$ and $W_t = W_s + W^1_{\rm xc}$. The inverse of $[\mathbf{M}_t]$ is:

$$[\mathbf{M}_t]^{-1} = \frac{1}{mn}[\mathbf{I}] - \frac{1}{(mn + W_t q^2)(mn + R_t q_\perp^2 + W_t q^2)} R_t q_\perp^2 [\mathbf{O}_2] - \frac{1}{mn(mn + W_t q^2)} W_t q^2 [\mathbf{O}_3]. \tag{4.12}$$

A straightforward derivation leads to:

$$(\boldsymbol{U}_s + \boldsymbol{U}^1_{\rm xc})^t[\mathbf{M}_t]^{-1}(\boldsymbol{U}_s + \boldsymbol{U}^1_{\rm xc})^* = \frac{\left(\frac{\hbar}{mn\lambda}X(mn + R_s q_\perp^2 + W_s q^2) + q_\perp \frac{\partial^2 e^1_{\rm xc}}{\partial n \partial \omega}\right)^2}{mn + R_t q_\perp^2 + W_t q^2} \tag{4.13}$$

and similarly, for the kinetic contribution alone:

$$(\boldsymbol{U}_s)^t[\mathbf{M}_s]^{-1}(\boldsymbol{U}_s)^* = \left(\frac{\hbar}{mn\lambda}X\right)^2 (mn + R_s q_\perp^2 + W_s q^2). \tag{4.14}$$

Finally, the current contribution to the effective local-field factor is:

$$Q_u(\boldsymbol{q}) = \left(\frac{\hbar}{mn\lambda}X\right)^2 (mn + R_s q_\perp^2 + W_s q^2) - \frac{\left[\frac{\hbar}{mn\lambda}X(mn + R_s q_\perp^2 + W_s q^2) + q_\perp \frac{\partial^2 e^1_{\rm xc}}{\partial n \partial \omega}\right]^2}{mn + R_t q_\perp^2 + W_t q^2} \tag{4.15}$$

which vanishes if $e^1_{\rm xc}$ does not depend on ω.

5. Applications

We have performed two types of applications of the previous study. First, the effective local-field factor has been systematically computed for densities in the metallic range $1 \leqslant r_s \leqslant 5$ and magnetic fields $0 \leqslant B/B_0 \leqslant 1$, where B_0 is the reference field (1 atomic unit of field is 2.35×10^9 Gauss). Then, we have applied the linear-response theory to the calculation of the equation of state of metallic aluminium in the presence of a magnetic field, in the domain of densities where the use of a standard weak model potential with valence $Z^* = 3$ is possible.

5.1. Numerical study of the effective local-field factor

The local-field factor $Q_u(\boldsymbol{q})$ defined in equation (4.15) has been calculated as a function of the variables $q_\perp$ and q, in the range $q\lambda \leqslant 10$. The angle θ between $\boldsymbol{q}$ and the z-axis (in the direction of B) has been sampled in 54 values from 0 to π. For a simpler graphical display of the results, we have calculated the angular average:

$$\langle Q_u(\boldsymbol{q})\rangle = \tfrac{1}{2}\int_0^\pi Q_u(\boldsymbol{q}) \sin\theta \, {\rm d}\theta.$$

Figure 1 shows the variations of $\langle Q_u(\boldsymbol{q})\rangle$ for $r_s = 4$ and for field values $B/B_0 = 0.1$, 0.2, 0.3, 0.5 and 1. For all these fields, only the first Landau band ($N = 0$) is populated. One sees that:

(1) The variations with respect to $q\lambda$ for a fixed B are not monotonous; $\langle Q_u(\boldsymbol{q})\rangle$ tends towards a constant limit for large values of $q\lambda$.

(2) The variations with respect to B for a fixed $q\lambda$ are not monotonous.

(3) The sign is not constant. The part Q_n of the local-field factor associated with the density change of the xc potential is always negative, but this is not true for $Q_u(\boldsymbol{q})$.

The accidents on the curves, particularly for $B/B_0 = 0.2$, are due to the logarithmic singularities of the function $\mathrm{G}_{MN}(t)$ mentioned in section 2.3 (here for $M = N = 0$). We will return to this point later.

The influence of the density is illustrated by moving to $r_s = 2$. The variations of $\langle Q_u(\boldsymbol{q})\rangle$ for five values of the field $B/B_0 = 0.1$, 0.2, 0.3, 0.5 and 1 are displayed in figure 2. Now, the index of the band containing the Fermi level is no longer always the

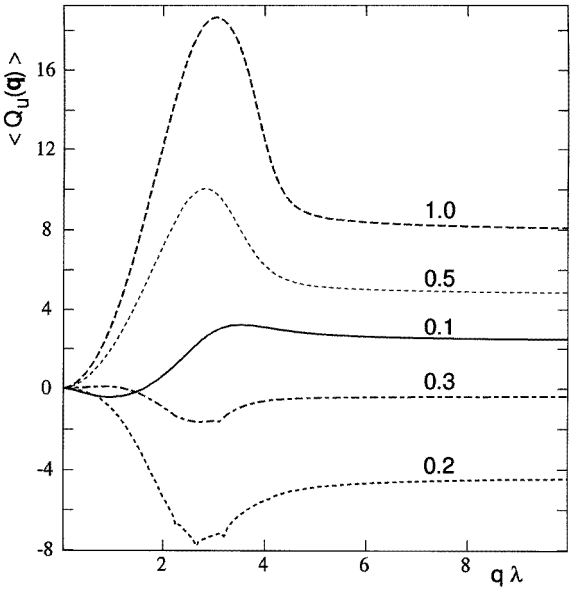

Figure 1. Current contribution to the local field factor, averaged over the angle between $\boldsymbol{B}$ and $\boldsymbol{q}$, as a function of $q\lambda$ (λ is the magnetic length) for several values of the magnetic field (0.1, 0.2, 0.3, 0.5 and 1, in units of B_0). Density: $r_s = 4$.

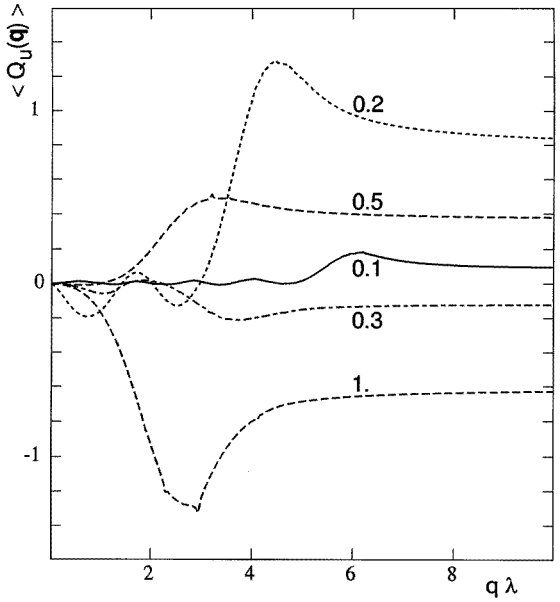

Figure 2. Current contribution to the local field factor, averaged over the angle between $\boldsymbol{B}$ and $\boldsymbol{q}$, as a function of $q\lambda$ (λ is the magnetic length) for several values of the magnetic field (0.1, 0.2, 0.3, 0.5 and 1, in units of B_0). Density: $r_s = 2$.

Table 1. The value (independent of q) of the density contribution Q_n to the local field factor, and the asymptotic value of the current contribution Q_u (averaged over the angle between $\boldsymbol{B}$ and $\boldsymbol{q}$) to the local field factor, for various values of the density parameter r_s and of the magnetic field B.

r_s	B/B_0	Q_n	$\langle Q_u(\boldsymbol{q})\rangle$
2	0.1	−3.62	0.095
	0.2	−3.26	0.842
	0.3	−3.70	−0.121
	0.5	−3.59	0.379
	1.0	−3.75	−0.628
4	0.1	−14.43	+2.48
	0.2	−16.39	−4.46
	0.3	−14.89	−0.41
	0.5	−13.30	+4.86
	1.0	−13.20	+8.09

same. This index is $N = 0$ for $B/B_0 = 1$ and 0.5, $N = 1$ for $B/B_0 = 0.3$ and 0.2 and $N = 4$ for $B/B_0 = 0.1$. We see that, for this density, several extrema in the variations of $\langle Q_u(\boldsymbol{q})\rangle$ as a function of $q\lambda$ may exist.

In order to compare the relative importance of the two contributions Q_n and Q_u to the local field factor, in table 1 we give the value (independent of q) of Q_n and the quasi-asymptotic value of $\langle Q_u(\boldsymbol{q})\rangle$ (for $q\lambda = 10$).

The interacting response function to be used in the calculation of the induced density is $\tilde{\chi}_{nV}(\boldsymbol{q})$, as defined in equation (4.4), with $Q(\boldsymbol{q})$ calculated in the local approximation of $E_{\rm xc}$, as shown above. We have found that this response function may have, for particular values of the parameters, one or several poles. Such a situation does not occur in the absence of a magnetic field. In order to understand the origin of these poles, let us consider the denominator of $\tilde{X}_{nV}(\boldsymbol{q})$ that can be written:

$$1 + \left(\frac{4\pi}{q^2} + Q(\boldsymbol{q})\right)|\chi_{nV}(\boldsymbol{q})|.$$

It has been seen that Q_u can be negative and therefore enhance the effect of Q_n. In addition, there are values of q_z for which $|\chi_{nV}(\boldsymbol{q})|$ has a logarithmic singularity and becomes infinite. If $4\pi/q^2 + Q(\boldsymbol{q})$ is also negative in the neighbourhood of the singularity, then the denominator can vanish. Figure 3 shows the variations of $\langle\tilde{\chi}_{nV}(\boldsymbol{q})\rangle$ (the average is over the angle of $\boldsymbol{q}$) for $r_s = 4$ and four values of the magnetic field $B/B_0 = 0.1$, 0.2, 0.5 and 1. For $B/B_0 = 0.2$, poles of $\tilde{X}_{nV}(\boldsymbol{q})$ do exist, which give rise to the spikes that are seen in figure 3.

The systematic search for poles of $\tilde{X}_{nV}(\boldsymbol{q})$, as functions of r_s, B, q and q_z is quite intricate. We have found that the domain where poles do exist is approximately bound by:

$$r_s \geqslant 3.50 \qquad \text{and} \qquad 0.3 \geqslant B/B_0 \geqslant 0.1.$$

The values of q involved are in general in the range $3 \geqslant q\lambda \geqslant 1$. Figure 4 corresponding to $r_s = 2$ shows that there is no pole in this case. It seems that the Fermi level is always in the first Landau band ($N = 0$) when a pole appears.

The existence of values of $\boldsymbol{q}$ for which the density $\delta n(\boldsymbol{q})$ becomes infinite (which would imply collective density oscillations in space) is likely a non-physical consequence of the approximations made. Several causes may be invoked.

(1) The accuracy of the numerical fit of $E_{\rm xc}^1$ in the strong-field regime (bottom of the first Landau band) and in particular the variation like $1/r_s$ discussed by Skudlarski and

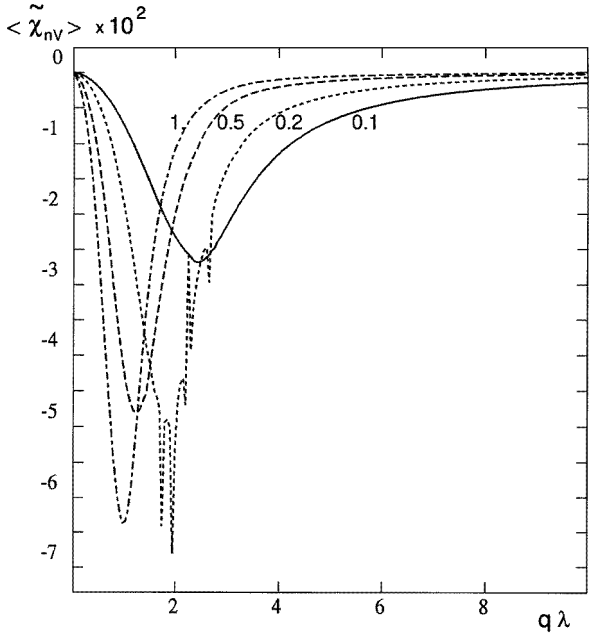

Figure 3. Density/scalar potential interacting response function, averaged over the angle between $\boldsymbol{B}$ and $\boldsymbol{q}$, as a function of $q\lambda$ (λ is the magnetic length) for several values of the magnetic field (0.1, 0.2, 0.5 and 1, in units of B_0). Density: $r_s = 4$.

Vignale [59]. Any inaccuracy in $E_{\rm xc}$ can produce much larger inaccuracies in the second derivatives which enter the local-field factor.

(2) The RPA approximation for $E^1_{\rm xc}$.

(3) The use of the local approximation for $E_{\rm xc}$, which discards any q-dependence of the derivatives with respect to density and current, although the local approximation is in principle good for strong magnetic fields (short magnetic lengths λ).

(4) The omission of spin polarization because the polarized version of $E^1_{\rm xc}$ is not available.

In conclusion, the numerical results show that the use of the linear response method in conjunction with the xc local-density approximation cannot be considered as reliable for density parameters $r_s \geqslant 3.50$. The true origin of the problem remains to be understood. Also, it would be useful to know whether this drawback could be overcome with a better knowledge of $E_{\rm xc}$.

5.2. Equation of state of aluminium

We now present results for the total energy and pressure of an aluminium atom, in a domain of densities where linear response theory can be applied together with a local model potential for electron–ion interaction. The aluminium atom is here embedded in a jellium without accounting for the periodic structure of the lattice which leads, in the presence of a magnetic field, to mathematical complexity outside the scope of this study [64].

We first consider a jellium with uniform density n. The unperturbed energy of the

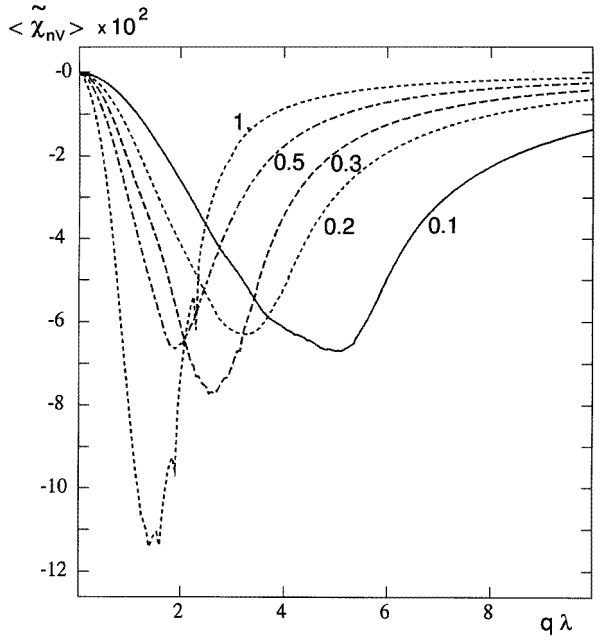

Figure 4. Density/scalar potential interacting response function, averaged over the angle between $\boldsymbol{B}$ and $\boldsymbol{q}$, as a function of $q\lambda$ (λ is the magnetic length) for several values of the magnetic field (0.1, 0.2, 0.3, 0.5 and 1, in units of B_0). Density: $r_s = 2$.

valence electrons ($Z^* = 3$) is:

$$E_u = \frac{Z^*}{n}\left(e_s(n,\omega) + e^1_{\mathrm{xc}}(n,\omega)\right) \tag{5.1}$$

where $e_s(n,\omega)$ is given by equation (2.26) and where $e^1_{\mathrm{xc}}(n,\omega)$ is the xc energy in the approximation of Skudlarski and Vignale. Then, a spherical cavity $n_a(r)$ with radius R_a equal to the atomic radius, and with charge Z^*, is introduced into the jellium. An aluminium ion is put at the centre of the cavity. This ion is modelled by the potential [65]:

$$V_{ps} = -\frac{4\pi Z^* e^2}{q^2}\cos(qR_c)\exp(-(q/q_0)^2) \tag{5.2}$$

where R_c is the core radius. The effect of the exponential factor is to cut the large $\boldsymbol{q}$-vectors. The numerical values are: $R_c = 1.367$ au and $q_0 = 5$ au. The cavity itself creates a perturbing potential which is, in Fourier space:

$$V_{\mathrm{cav}} = \frac{4\pi Z^* e^2}{q^2} f(qR_a) \tag{5.3a}$$

$$f(qR_a) = 3\frac{\sin(qR_a) - qR_a\cos(qR_a)}{(qR_a)^3}. \tag{5.3b}$$

The total external potential is therefore: $V_{\mathrm{ext}} = V_{ps} + V_{\mathrm{cav}}$. This potential V_{ext} is short ranged and induces a charge density $\delta n(\boldsymbol{r})$ which integrates to zero. The perturbation is weak and hence use of the linear response method is justified. The perturbation of the order 1 and 2 are:

$$E_1 = n\int V_{\mathrm{ext}}(r)\,\mathrm{d}^3 r \tag{5.4a}$$

which can be calculated analytically:

$$E_1 = 4\pi Z^* e^2 \left(\frac{1}{2} R_c^2 + \frac{1}{q_0^2} - \frac{1}{10} R_a^2 \right) \tag{5.4b}$$

and:

$$E_2 = \tfrac{1}{2} \int V_{\text{ext}}(q) \tilde{\chi}_{nV}(\boldsymbol{q}) V_{\text{ext}}(q) \, \mathrm{d}^3 q. \tag{5.5}$$

The change in the ion–ion interaction energy is:

$$E_{ii} = \frac{1}{2} \int (n - n_a(r)) \frac{e^2}{|\boldsymbol{r} - \boldsymbol{r}'|} (n - n_a(r)) \, \mathrm{d}^3 r \, \mathrm{d}^3 r' - \frac{1}{2} \int n \frac{e^2}{|\boldsymbol{r} - \boldsymbol{r}'|} n \, \mathrm{d}^3 r \, \mathrm{d}^3 r' + \int (n - n_a(r)) \frac{Z^* e^2}{r} \, \mathrm{d}^3 r \tag{5.6a}$$

which is easily calculated:

$$E_{ii} = -\frac{3}{5} \frac{Z^{*2} e^2}{R_a}. \tag{5.6b}$$

Adding all the previous contributions, one obtains the binding energy of the aluminium atom in the SMEG:

$$E_b = E_u + E_1 + E_2 + E_{ii}. \tag{5.7}$$

So far the effect of the magnetic field on the internal structure of the Al^{+3} ion, whose configuration is $1s^2\,2s^2\,2p^6$, has been ignored. This effect for values of the field considered here must now be investigated. The perturbing one-electron Hamiltonian for the core states is:

$$\Delta H = -\frac{1}{2} \mathrm{i} \bar{h} \omega \frac{\partial}{\partial \varphi} + \frac{1}{8} m \omega^2 r^2 \cos^2 \theta. \tag{5.8}$$

φ and θ are the common angles of the position vector with respect to the axes. We have diagonalized this perturbation in the subspace spanned by the one-electron wavefunctions of the aluminium ground state (1s, 2s, 2p, 3s and 3p). These wavefunctions were calculated for zero field with a self-consistent atomic structure program solving the Kohn–Sham equations with an xc potential in the local-density approximation. We have found that the shift of the core levels 1s, 2s and 2p is reproduced to an excellent accuracy (better than 3×10^{-4} Rydberg) by a first-order perturbation calculation, for magnetic fields $B \leqslant B_0$. Hence, the change in the core wavefunctions is negligible. The energy perturbation due to the magnetic field can be calculated to first order:

$$E_{c0} = \tfrac{1}{8} m \omega^2 [\tfrac{2}{3} \langle r^2 \rangle_{2\text{s}} + 2 \langle r^2 \rangle_{2\text{p}}] \tag{5.9}$$

in terms of the average square of the radii in shells 2s and 2p. The 1s contribution is negligible. The contributions linear in ω for the 2p $m = 1$ and 2p $m = -1$ states cancel because the projections of the angular momentum are opposite. The magnetic corrections for core states being independent of the density, they do not contribute to the pressure.

In table 2, we give the equation of state results for magnetized aluminium. The compression is:

$$c = \left(\frac{r_{s0}}{r_s} \right)^3$$

Table 2. Equation of state of magnetized aluminium, as a function of the electron density parameter r_s, from 1.72 to 2.12. E is the binding energy per atom (Rydbergs), P the pressure (Mbars) and y the reduced Fermi energy $\frac{\mu}{\hbar\omega} - \frac{1}{2}$.

B/B_0		1.72	1.77	1.82	1.87	1.92	1.97	2.02	2.07	2.12
0.0	$-E$	3.7739	3.8355	3.8812	3.9141	3.9366	3.9507	3.9581	3.9602	3.9581
	P	1.880	1.334	0.924	0.616	0.387	0.216	0.091	−0.001	−0.066
0.1	$-E$	3.7503	3.8152	3.8681	3.8929	3.9161	3.9330	3.9439	3.9416	3.9395
	P	1.780	1.473	1.115	0.561	0.423	0.279	0.111	−0.031	−0.064
	y	5.745	5.351	5.068	4.806	4.472	4.216	4.039	3.856	3.589
0.2	$-E$	3.7105	3.7860	3.8442	3.8899	3.9289	—	3.8919	3.9025	3.9048
	P	2.179	1.662	1.222	0.942	0.835	—	0.259	0.117	−0.020
	y	2.607	2.396	2.235	2.115	2.035	2.000	1.826	1.659	1.521
0.3	$-E$	3.6742	3.7459	3.7969	3.8315	3.8546	3.8697	3.8804	3.8884	—
	P	2.190	1.524	1.007	0.642	0.403	0.259	0.179	0.123	—
	y	1.556	1.411	1.296	1.205	1.135	1.082	1.044	1.018	1.003
0.5	$-E$	3.5880	3.6099	3.6449	3.6716	3.6854	3.6871	3.6776	3.6587	3.6329
	P	−0.278	0.855	0.768	0.451	0.164	−0.079	−0.272	−0.406	−0.495
	y	0.858	0.722	0.611	0.519	0.443	0.380	0.327	0.282	0.213
1.0	$-E$	2.8557	2.8401	2.8113	2.7688	2.7138	2.6535	2.5830	2.5111	2.4404
	P	−0.013	−0.552	−0.838	−1.075	−1.223	−1.313	−1.340	−1.317	−1.255
	y	0.128	0.090	0.076	0.065	0.055	0.047	0.041	0.035	0.031

with r_{s0} the equilibrium density parameter for the zero magnetic field, that is $r_{s0} = 2.07$. The energy tabulated is:

$$E = E_b + E_{c0}$$

where E is the total energy of the magnetized atom in the jellium minus the energy of the ion at zero field. The energies are in Rydberg units and the pressures in Mbars. We give also the quantity:

$$y = \frac{\mu}{\hbar\omega} - \frac{1}{2}$$

whose integer part is the index of the Landau band where the Fermi level is located.

For the magnetic field $B = 0.1B_0$, the Fermi level lies, depending on the density, in the band of index $N = 5$, 4 or 3. For $B = 0.2B_0$, it is in the $N = 2$ or 1 band. For $B = 0.3B_0$, it is still in the $N = 1$ band, and for larger values of the field, it is always in the lowest band, $N = 0$.

The variations of pressure with density are shown in figure 5. The discussion in section 4 has shown that the linear response method is not valid when the highest occupied Landau band is nearly filled or empty. This corresponds to the ranges of densities where there are no results in the tables (indicated by —) and where the curves break off. To our knowledge, at the present time there is no theory able to treat properly the equation-of-state problem for these values of the couple density-magnetic field. The results show a non-monotonous behaviour of the pressure as a function of volume, particularly for $B = 0.5B_0$. They also indicate that the pressure can become negative for volumes where it is positive without a field. This means that the magnetized atom shrinks and its charge density is much more

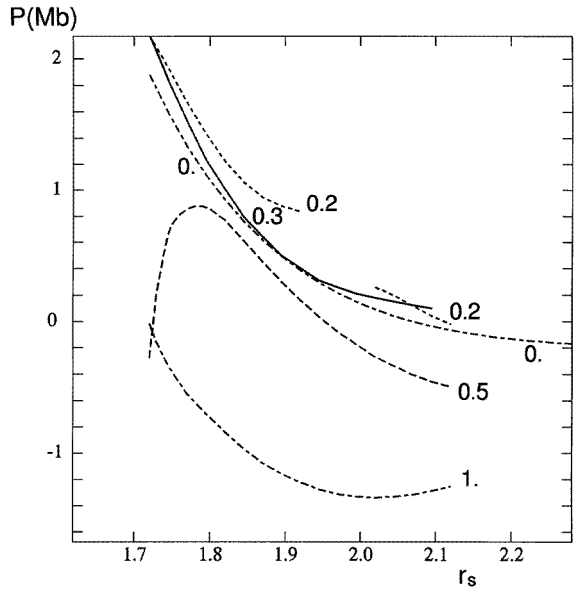

Figure 5. Pressure in metallic aluminium, as a function of the density parameter r_s, for magnetic fields between 0 and 1, in units of B_0.

localized. It behaves as the atom without a field for a larger volume. For $B = B_0$ for instance, the equilibrium radius is $r_s = 1.72$ instead of 2.07 for a zero field.

6. Conclusion

We have studied the properties linked with the linear response of the uniform electron gas in the presence of a strong magnetic field. In the non-interacting case, we have given closed-form expressions for the three independent response functions: (i) χ_{nV} which gives the density induced by a scalar potential, (ii) χ_{JV} which gives the current induced by a scalar potential, (iii) $[\chi_{JA}]$ which gives the current induced by a vector potential. Then it has been shown that, in the interacting case, the exchange and correlation effects, which depend also on the paramagnetic current, introduce the response functions χ_{JV} and $[\chi_{JA}]$ into the effective local-field factor included in the $\tilde{\chi}_{nV}$, even when the external perturbation is purely scalar.

The xc effects have been accounted for in the local-density approximation, using the only known form $E^1_{\rm xc}(n,\omega)$ of the energy functional for the SMEG. The interacting response function $\tilde{\chi}_{nV}(\boldsymbol{q})$ is singular when the Fermi level coincides with a Landau band edge. The numerical study of the effective local-field factor shows that this response function can also have poles in a particular region of the plane density-magnetic field ($r_s > 3.5$ and $0.3 \geqslant B/B_0 \geqslant 0.1$). This is probably a non-physical consequence of the approximations made. But this point deserves further theoretical investigation. Were the existence of such poles shown to be independent of the approximation used for $E_{\rm xc}$, then the local-density approximation would not be valid in such magnetized systems.

Restricting to a region of the density-magnetic field plane outside the domain indicated above, we have applied the linear response method to the study of the equation of state of aluminium. The densities treated are in the range where the linear response method with a

simple model potential is of common use in the absence of a magnetic field (compressions going from 0.8 to 1.5). The magnetic fields considered reach the value $B = B_0$, or 2.35×10^9 Gauss. The results show the importance of the modifications induced by the magnetic field, in particular those resulting from electron-charge density localization.

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