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A Rigorous Proof of the Landau-Peierls Formula and much more

Philippe Briet, Horia D. Cornean and Baptiste Savoie

Abstract. We present a rigorous mathematical treatment of the zero-field orbital magnetic susceptibility of a non-interacting Bloch electron gas, at fixed temperature and density, for both metals and semiconductors/insulators. In particular, we obtain the Landau-Peierls formula in the low temperature and density limit as conjectured by Kjeldaas and Kohn (Phys Rev 105:806–813, 1957).

1. Introduction and the Main Results

Understanding the zero-field magnetic susceptibility of a Bloch electron gas is one of the oldest problems in quantum statistical mechanics.

The story began in 1930 with a paper by Landau [30], in which he computed the diamagnetic susceptibility of a free degenerate gas. (Note that the rigorous proof of Landau's formula for free electrons was given by Angelescu et al. [1] and came as late as 1975). For Bloch electrons (which are subjected to a periodic background electric potential), the problem is much harder and—to our best knowledge—it has not been solved yet in its full generality.

The first important contribution to the periodic problem came, when Peierls [34] introduced his celebrated Peierls substitution and constructed an effective band Hamiltonian which permitted to reduce the problem to free electrons. Needless to say that working with only one energy band instead of the full magnetic Schrödinger operator is an important simplification. Under the tight-binding approximation he claimed that the dominant contribution to the zero-field orbital susceptibility of a Bloch electron gas in metals (at zero temperature) is purely diamagnetic and is given by the so-called Landau-Peierls formula which consists of replacing in the Landau formula the mass by the effective mass of the electron. He showed as well the existence of another contribution which has no simple interpretation and whose magnitude and sign are uncertain.

Adams [2] claimed that the Landau-Peierls susceptibility is not always the dominant contribution to the zero-field orbital susceptibility. By considering the case of 'simple metals' (for which the tight-binding approximation is not appropriate), he showed that there exist other contributions (certain having even positive sign!) coming from bands not containing the Fermi energy. Besides some special cases, these contributions are of the same order of magnitude as the one given by the Landau-Peierls formula. However, no general formulas of these other contributions were given.

Kjeldaas and Kohn [26] were probably the first ones who suggested that for 'simple metals' *the Landau-Peierls approximation is only valid in the limit of weak density of electrons*, and moreover, the Landau-Peierls formula (see below (1.17) and (1.18)) has to be corrected with some higher order terms in the particle density, and these terms must come from the bands not containing the Fermi energy.

These three papers generated a lot of activity, where the goal was to write down an exact expression for the zero-field magnetic susceptibility of a Bloch electron gas in metals at zero temperature. In what follows we comment on some of the most important works.

The first attempt to address the full quantum mechanical problem—even though the carriers were boltzons and not fermions—was made by Hebborn and Sondheimer [21,22]. Unlike the previous authors, they developed a magnetic perturbation theory for the trace per unit volume defining the pressure. The biggest problem of their formalism is that they assumed that all Bloch energy bands are not overlapping (this is generically false; for a proof of the Bethe–Sommerfeld conjecture in dimension 3 see e.g. [23]), and that the Bloch basis is smooth in the quasi-momentum variables. This assumption can fail at the points where the energy bands cross each other. Not to mention that no convergence issues were addressed in any way.

Roth [36] developed a sort of magnetic pseudodifferential calculus starting from the ideas of Peierls, Kjeldaas and Kohn. She used this formalism in order to compute local traces and magnetic expansions. Similar results are obtain by Blunt [9]. Their formal computations can most probably be made rigorous in the case of simple bands.

Hebborn et al. [20] simplified the formalism developed in [22] and gave for the first time a formula for the zero-field susceptibility of a boltzon gas. Even though the proofs lack any formal rigor, we believe that their derivation could be made rigorous for systems where the Bloch bands do not overlap. But this is generically not the case.

The same year, Wannier and Upadhyaya [40] go back to the method advocated by Peierls, and replace the true magnetic Schrödinger operator with a (possibly infinite) number of bands modified with the Peierls phase factor. They claim that their result is equivalent with that one of Hebborn and Sondheimer [22], but no details are given. Anyhow, the result uses in an essential way the non-overlapping of Bloch bands. At the same time, Glasser [18] gave an expression of the bulk zero-field susceptibility in terms of effective mass by the usual nearly free electron approximation.

Misra and Roth [32] combined the method of [36] with the ideas of Wannier in order to include the core electrons in the computation.

Misra and Kleinman [31] had the very nice idea of using sum-rules in order to replace derivatives with respect to the quasi-momentum variables, with matrix elements of the "true" momentum operator. They manage in this way to rewrite the formulas previously derived by Misra and Roth (which only made sense for non-overlapping bands) in a form which might also hold for overlapping bands.

As we have already mentioned, the first serious mathematical approach on the zero-field susceptibility appeared as late as 1975, due to Angelescu et al. [1]. Then, Helffer and Sjöstrand [24] developed for the first time a rigorous theory based on the Peierls substitution and considered the connection with the de Haas–Van Alphen effect. These and many more results were reviewed by Nenciu [33]. A related problem in which the electron gas is confined by a trapping potential was considered by Combescure and Robert [11]. They obtained the Landau formula in the limit $\hbar \to 0$.

Finally we mention that the magnetic response can be described using the semiclassical theory of the orbital magnetism and the Berry-phase formula, see [35] for further details. The link between this approach and our work has yet to be clarified.

Our current paper is based on what we call magnetic perturbation theory, as developed by the authors and their collaborators in a series of papers starting with 2000 (see [3–7,12–16] and references therein). The results we obtain in Theorem 1.2 give a complete answer to the problem of zero-field susceptibility. Let us now discuss the setting and properly formulate the mathematical problem.

1.1. The Setting

Consider a confined quantum gas of charged particles obeying the Fermi–Dirac statistics. The spin is not considered since we are only interested in orbital magnetism. Assume that the gas is subjected to a constant magnetic field and an external periodic electric potential. The interactions between particles are neglected and the gas is at thermal equilibrium.

The gas is trapped in a large cubic box, which is given by $\Lambda_L = (-\frac{L}{2}, \frac{L}{2})^3, L \geq 1$.

Let us introduce our one-body Hamiltonian. We consider a uniform magnetic field $\mathbf{B} = (0, 0, B)$ with $B \geq 0$, parallel to the third direction of the canonical basis of $\mathbb{R}^3$. Let $\mathbf{a}(\mathbf{x})$ be the symmetric (transverse) gauge $\mathbf{a}(\mathbf{x}) := \frac{1}{2}(-x_2, x_1, 0)$ which generates the magnetic field $(0, 0, 1)$.

We consider that the background electric potential V is smooth, i.e. $V \in \mathcal{C}^\infty(\mathbb{R}^3)$ is a real-valued function and periodic with respect to a (Bravais) lattice Υ with unit cell Ω. Without loss of generality, we assume that Υ is the cubic lattice $\mathbb{Z}^3$, thus Ω is the unit cube centered at the origin of coordinates.

When the box is finite i.e. $1 \leq L < \infty$, the dynamics of each particle is determined by a Hamiltonian defined in $L^2(\Lambda_L)$ with Dirichlet boundary conditions on $\partial\Lambda_L$:

$$H_L(\omega) = \frac{1}{2}\left(-i\nabla_{\mathbf{x}} - \omega\mathbf{a}(\mathbf{x})\right)^2 + V_L(\mathbf{x}) \tag{1.1}$$

where V_L stands for the restriction of V to the box Λ_L. Here $\omega := \frac{e}{c}B \in \mathbb{R}$ denotes the cyclotron frequency. The operator $H_L(\omega)$ is self-adjoint on the domain $D(H_L(\omega)) = \mathcal{H}_0^1(\Lambda_L) \cap \mathcal{H}^2(\Lambda_L)$. It is well known (see [37]) that $H_L(\omega)$ is bounded from below and has compact resolvent. This implies that its spectrum is purely discrete with an accumulation point at infinity. We denote the set of eigenvalues (counting multiplicities and in increasing order) by $\{e_j(\omega)\}_{j\geq 1}$.

When $L = \infty$ we denote by $H_\infty(\omega)$ the unique self-adjoint extension of the operator

$$\frac{1}{2}\left(-i\nabla_{\mathbf{x}} - \omega\mathbf{a}(\mathbf{x})\right)^2 + V(\mathbf{x}) \tag{1.2}$$

initially defined on $\mathcal{C}_0^\infty(\mathbb{R}^3)$. Then $H_\infty(\omega)$ is bounded from below and only has essential spectrum (see e.g. [8]).

Now let us define some quantum statistical quantities related to the quantum gas introduced above. For the moment we use the grand canonical formalism. The finite volume pressure and density of our quantum gas at inverse temperature $\beta := (k_B T)^{-1} > 0$ (k_B stands for the Boltzmann constant), at fugacity $z := \mathrm{e}^{\beta\mu} > 0$ ($\mu \in \mathbb{R}$ stands for the chemical potential) and at cyclotron frequency $\omega \in \mathbb{R}$ are given by (see e.g. [19]):

$$\begin{aligned} P_L(\beta, z, \omega) &:= \frac{1}{\beta|\Lambda_L|}\mathrm{Tr}_{L^2(\Lambda_L)}\left\{\ln\left(\mathbf{1} + z\mathrm{e}^{-\beta H_L(\omega)}\right)\right\} \\ &= \frac{1}{\beta|\Lambda_L|}\sum_{j=1}^{\infty}\ln\left(1 + z\mathrm{e}^{-\beta e_j(\omega)}\right) \end{aligned} \tag{1.3}$$

$$\rho_L(\beta, z, \omega) := \beta z \frac{\partial P_L}{\partial z}(\beta, z, \omega) = \frac{1}{|\Lambda_L|}\sum_{j=1}^{\infty}\frac{z\mathrm{e}^{-\beta e_j(\omega)}}{1 + z\mathrm{e}^{-\beta e_j(\omega)}}. \tag{1.4}$$

As the semi-group $\mathrm{e}^{-\beta H_L(\omega)}$ is trace class, the series in (1.3) and (1.4) are absolutely convergent. Since the function $\mathbb{R} \ni \omega \mapsto P_L(\beta, z, \omega)$ is smooth (see [7]), we can define the finite volume orbital susceptibility as the second derivative of the pressure with respect to the intensity B of the magnetic field at $B = 0$ (see e.g. [1]):

$$\mathcal{X}_L^{GC}(\beta, z) := \left(\frac{\mathrm{e}}{c}\right)^2 \frac{\partial^2 P_L}{\partial \omega^2}(\beta, z, 0). \tag{1.5}$$

When Λ_L fills the whole space, we proved in [39] that the thermodynamic limits of the three grand canonical quantities defined above exist. By denoting $P_\infty(\beta, z, \omega) := \lim_{L\to\infty} P_L(\beta, z, \omega)$, we proved moreover the following pointwise convergence:

$$\rho_\infty(\beta, z, \omega) := \beta z \frac{\partial P_\infty}{\partial z}(\beta, z, \omega) = \lim_{L\to\infty} \beta z \frac{\partial P_L}{\partial z}(\beta, z, \omega) \tag{1.6}$$

$$\mathcal{X}_\infty^{GC}(\beta, z) := \left(\frac{\mathrm{e}}{c}\right)^2 \frac{\partial^2 P_\infty}{\partial \omega^2}(\beta, z, 0) = \lim_{L\to\infty} \left(\frac{\mathrm{e}}{c}\right)^2 \frac{\partial^2 P_L}{\partial \omega^2}(\beta, z, 0) \tag{1.7}$$

and the limit commutes with the first derivative (resp. the second derivative) of the grand canonical pressure with respect to the fugacity z (resp. to the external magnetic field B).

Now assume that our fixed external parameter is the density of particles $\rho_0 > 0$. We prefer to see ρ_∞ as a function of the chemical potential μ instead of the fugacity z; the density is a strictly increasing function with respect to both μ and z. Denote by $\mu_\infty(\beta, \rho_0) \in \mathbb{R}$ the unique solution of the equation:

$$\rho_0 = \rho_\infty\left(\beta, \mathrm{e}^{\beta\mu_\infty(\beta,\rho_0)}, 0\right). \tag{1.8}$$

The bulk orbital susceptibility at $\beta > 0$ and fixed density $\rho_0 > 0$ defined from (1.7) is defined as:

$$\mathcal{X}(\beta, \rho_0) := \mathcal{X}_\infty^{GC}\left(\beta, \mathrm{e}^{\beta\mu_\infty(\beta,\rho_0)}\right). \tag{1.9}$$

In fact one can also show that $\mathcal{X}(\beta, \rho_0) = -(\frac{\mathrm{e}}{c})^2 \frac{\partial^2 f_\infty}{\partial\omega^2}(\beta, \rho_0, 0)$ where $f_\infty(\beta, \rho_0, \omega)$ is the thermodynamic limit of the reduced free energy defined as the Legendre transform of the thermodynamic limit of the pressure (see e.g. [38]). Note that for a perfect quantum gas and in the limit of low temperatures, (1.9) leads to the so-called Landau diamagnetic susceptibility, see e.g. [1].

In order to formulate our main result, we need to introduce some more notation. In the case in which $\omega = 0$, the Floquet theory for periodic operators (see e.g. [10], [29] and Sect. 3) allows one to use the band structure of the spectrum of $H_\infty(0)$. Denote by $\Omega^* = 2\pi\Omega$ the Brillouin zone of the dual lattice $\Upsilon^* \equiv 2\pi\mathbb{Z}^3$.

If $j \geq 1$, the jth Bloch band function is defined by $\mathcal{E}_j := [\min_{\mathbf{k}\in\Omega^*} E_j(\mathbf{k}), \max_{\mathbf{k}\in\Omega^*} E_j(\mathbf{k})]$ where $\{E_j(\mathbf{k})\}_{j\geq 1}$ is the set of eigenvalues (counting multiplicities and in *increasing* order) of the fiber Hamiltonian $h(\mathbf{k}) := \frac{1}{2}(-i\nabla + \mathbf{k})^2 + V$ living in $L^2(\mathbb{T}^3)$ with $\mathbb{T}^3 := \mathbb{R}^3/\mathbb{Z}^3$ the 3-dimensional torus. With this definition, the Bloch energies $E_j(\cdot)$ are continuous on the whole of Ω^*, but they are differentiable only outside a zero Lebesgue measure subset of Ω^* corresponding to cross-points. In the following we make the assumption that the E_j's are simple eigenvalues for $\mathbf{k}$ in a subset of Ω^* with full measure. Note that this assumption is not essential for our approach but it simplifies the presentation, see Remark 3 below the Theorem 1.2.

The spectrum of $H_\infty(0)$ is absolutely continuous and given (as a set of points) by $\sigma(H_\infty(0)) = \bigcup_{j=1}^\infty \mathcal{E}_j$. Note that the sets $\mathcal{E}_j$ can overlap each other in many ways, and some of them can even coincide even though they are images of increasingly ordered functions. The energy bands are disjoint unions of $\mathcal{E}_j$'s. Moreover, if $\max \mathcal{E}_j < \min \mathcal{E}_{j+1}$ for some $j \geq 1$ then we have a spectral gap. Since the Bethe-Sommerfeld conjecture holds true under our conditions [23], the number of spectral gaps is finite, if not zero.

It remains to introduce the integrated density of states of the operator $H_\infty(0)$. Recall its definition. For any $E \in \mathbb{R}$, let $N_L(E)$ be the number of eigenvalues of $H_L(0)$ not greater than E. The integrated density of states of $H_\infty(0)$ is defined by the limit (see [17]):

$$n_\infty(E) := \lim_{L\to\infty} \frac{N_L(E)}{|\Lambda_L|} = \lim_{L\to\infty} \frac{\mathrm{Tr}\left\{\chi_{(-\infty,E]}(H_L(0))\right\}}{|\Lambda_L|} \tag{1.10}$$

and $n_\infty(\cdot)$ is a positive continuous and non-decreasing function (see e.g. [10]). In this case one can express $n_\infty(E)$ with the help of the Bloch energies in the following way:

$$n_\infty(E) = \frac{1}{(2\pi)^3} \sum_{j\geq 1} \int_{\Omega^*} \chi_{[E_0,E]}(E_j(\mathbf{k}))\, \mathrm{d}\mathbf{k} \tag{1.11}$$

where $\chi_{[E_0,E]}(\cdot)$ is the characteristic function of the interval $[E_0, E]$. Thus n_∞ is clearly continuous in E due to the continuity of the Bloch bands. Moreover, this function is piecewise constant when E belongs to a spectral gap.

1.2. The Statements of our Main Results

The first theorem is not directly related to the magnetic problem, and it deals with the rigorous definition of the Fermi energy for Bloch electrons. Even though these results are part of the 'physics folklore', we have not found a serious mathematical treatment in the literature.

Theorem 1.1. *Let $\rho_0 > 0$ be fixed. If $\mu_\infty(\beta, \rho_0)$ is the unique real solution of the equation $\rho_\infty(\beta, \mathrm{e}^{\beta\mu}, 0) = \rho_0$ (see (1.8)), then the limit*:

$$\mathcal{E}_F(\rho_0) := \lim_{\beta\to\infty} \mu_\infty(\beta, \rho_0) \tag{1.12}$$

exists and defines an increasing function of ρ_0 called the Fermi energy. There can only occur two cases:

SC (*semiconductor/insulator/semimetal*): *Suppose that there exists some $N \in \mathbb{N}^*$ such that $\rho_0 = n_\infty(E)$ for all $E \in [\max \mathcal{E}_N, \min \mathcal{E}_{N+1}]$. Then:*

$$\mathcal{E}_F(\rho_0) = \frac{\max \mathcal{E}_N + \min \mathcal{E}_{N+1}}{2}. \tag{1.13}$$

M (*metal*): *Suppose that there exists a unique solution E_M of the equation $n_\infty(E_M) = \rho_0$ which belongs to $(\min \mathcal{E}_N, \max \mathcal{E}_N)$ for some (possibly not unique) N. Then:*

$$\mathcal{E}_F(\rho_0) = E_M. \tag{1.14}$$

Remark 1. In other words, a semiconductor/semimetal either has its Fermi energy in the middle of a non-trivial gap (this occurs if $\max \mathcal{E}_N < \min \mathcal{E}_{N+1}$), or where the two consecutive Bloch bands touch each other closing the gap (this occurs if $\max \mathcal{E}_N = \min \mathcal{E}_{N+1}$). As for a metal, its Fermi energy lies in the interior of a Bloch band.

Remark 2. According to the above result, $\mathcal{E}_F$ is discontinuous at all values of ρ_0 for which the equation $n_\infty(E) = \rho_0$ does not have a unique solution. Each open gap gives such a discontinuity.

Now here is our main result concerning the orbital susceptibility of a Bloch electrons gas at fixed density and zero temperature:

Theorem 1.2. *Denote by* $E_0 := \inf \sigma(H_\infty(0))$.

(i) *Assume that the Fermi energy is in the middle of a non-trivial gap (see (1.13)). Then there exist* $2N$ *functions* $\mathfrak{c}_j(\cdot), \mathfrak{d}_j(\cdot)$, *with* $1 \leq j \leq N$, *defined on* Ω^* *outside a set of Lebesgue measure zero, such that the integrand in (1.15) can be extended by continuity to the whole of* Ω^* *and:*

$$\mathcal{X}_{\mathrm{SC}}(\rho_0) := \lim_{\beta\to\infty} \mathcal{X}(\beta,\rho_0) = \left(\frac{\mathrm{e}}{c}\right)^2 \frac{1}{2}\frac{1}{(2\pi)^3} \int_{\Omega^*} \mathrm{d}\mathbf{k} \sum_{j=1}^{N} \left\{\mathfrak{c}_j(\mathbf{k}) + \{E_j(\mathbf{k}) - \mathcal{E}_F(\rho_0)\}\, \mathfrak{d}_j(\mathbf{k})\right\}. \tag{1.15}$$

(ii) *Suppose that there exists a unique* $N \geq 1$ *such that* $\mathcal{E}_F(\rho_0) \in (\min \mathcal{E}_N, \max \mathcal{E}_N)$. *Assume that the Fermi surface* $\mathcal{S}_F := \{\mathbf{k} \in \Omega^* : E_N(\mathbf{k}) = \mathcal{E}_F(\rho_0)\}$ *is smooth and non-degenerate. Then there exist* $2N+1$ *functions* $\mathcal{F}_N(\cdot), \mathfrak{c}_j(\cdot), \mathfrak{d}_j(\cdot)$ *with* $1 \leq j \leq N$, *defined on* Ω^* *outside a set of Lebesgue measure zero, in such a way that they are all continuous on* $\mathcal{S}_F$ *while the second integrand in (1.16) can be extended by continuity to the whole of* Ω^*:

$$\begin{aligned}\mathcal{X}_{\mathrm{M}}(\rho_0) &:= \lim_{\beta\to\infty} \mathcal{X}(\beta,\rho_0) = -\left(\frac{\mathrm{e}}{c}\right)^2 \frac{1}{12}\frac{1}{(2\pi)^3} \\ &\times \left\{ \int_{\mathcal{S}_F} \frac{\mathrm{d}\sigma(\mathbf{k})}{|\nabla E_N(\mathbf{k})|} \left[\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} - \left(\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2}\right)^2 - 3\mathcal{F}_N(\mathbf{k})\right] \right. \\ &\quad -6 \int_{\Omega^*} \mathrm{d}\mathbf{k} \sum_{j=1}^{N} \left[\chi_{[E_0,\mathcal{E}_F(\rho_0)]}(E_j(\mathbf{k}))\, \mathfrak{c}_j(\mathbf{k}) \right. \\ &\quad \left.\left. + \{E_j(\mathbf{k}) - \mathcal{E}_F(\rho_0)\}\, \chi_{[E_0,\mathcal{E}_F(\rho_0)]}(E_j(\mathbf{k}))\, \mathfrak{d}_j(\mathbf{k})\right] \right\}. \end{aligned} \tag{1.16}$$

Here $\chi_{[E_0,\mathcal{E}_F(\rho_0)]}(\cdot)$ *denotes the characteristic function of the interval* $E_0 \leq t \leq \mathcal{E}_F(\rho_0)$.

(iii) *Let* $k_F := (6\pi^2\rho_0)^{\frac{1}{3}}$ *be the Fermi wave vector. Then in the limit of small densities, (1.16) gives the Landau-Peierls formula:*

$$\mathcal{X}_{\mathrm{M}}(\rho_0) = -\frac{\mathrm{e}^2}{24\pi^2 c^2} \frac{(m_1^* m_2^* m_3^*)^{\frac{1}{3}}}{m_1^* m_2^*} k_F + o(k_F); \tag{1.17}$$

here $\left[\frac{1}{m_i^*}\right]_{1\leq i\leq 3}$ *are the eigenvalues of the positive definite Hessian matrix* $\{\partial_{ij}^2 E_1(\mathbf{0})\}_{1\leq i,j\leq 3}$.

Remark 1. The functions $\mathfrak{c}_j(\cdot)$ and $\mathfrak{d}_j(\cdot)$ with $1 \leq j \leq N$ which appear in (1.15) are the same as the ones in (1.16). All of them (as well as $\mathcal{F}_N(\cdot)$) can be explicitly written down in terms of Bloch energy functions and their associated eigenfunctions. One can notice in (1.16) the appearance of an explicit term associated with the Nth Bloch energy function; it is only this term which will generate the linear k_F behavior in the Landau-Peierls formula.

Remark 2. The functions $\mathfrak{c}_j(\cdot)$ and $\mathfrak{d}_j(\cdot)$ might have local singularities at a set of Lebesgue measure zero where the Bloch bands might touch each other. But their combinations entering the integrands above are always bounded because the individual singularities get canceled by the sum.

Remark 3. The results in (i) and (ii) hold true even if some Bloch bands are degenerate on a subset of full Lebesgue measure of Ω^*. But in this case the functions $\mathfrak{c}_j(\cdot), \mathfrak{d}_j(\cdot)$ and $\mathcal{F}_N(\cdot)$ cannot be expressed in the same way as mentioned in Remark 1. Their expressions are more complicated and require the use of the orthogonal projection corresponding to $E_j(\cdot)$, see the proof of Lemma 3.7 for further details.

Remark 4. When $m_1^* = m_2^* = m_3^* = m^*$ holds in (iii), (1.17) is nothing but the usual Landau-Peierls susceptibility formula:

$$\mathcal{X}_{\mathrm{M}}(\rho_0) \sim -\frac{\mathrm{e}^2}{24\pi^2 m^* c^2} k_F \quad \text{when } k_F \to 0. \tag{1.18}$$

Note that our expression is twice smaller than the one in [34] since we do not take into account the degeneracy related to the spin of the Bloch electrons.

Remark 5. The assumption $V \in \mathcal{C}^\infty(\mathbb{T}^3)$ can be relaxed to $V \in \mathcal{C}^r(\mathbb{T}^3)$ with $r \geq 23$. The smoothness of V plays an important role in the absolute convergence of the series defining $\mathcal{X}(\beta, \rho_0)$ in Theorem 3.1, before the zero-temperature limit; see [16] for a detailed discussion on sum rules and local traces for periodic operators.

Remark 6. The role of magnetic perturbation theory (see Sect. 3) is *crucial* when one wants to write down a formula for $\mathcal{X}(\beta, \rho_0)$ which contains no derivatives with respect to the quasi-momentum $\mathbf{k}$. Remember that the Bloch energies ordered in increasing order and their corresponding eigenfunctions are not necessarily differentiable at crossing points.

Remark 7. We do not treat the semi-metal case, in which the Fermi energy equals $\mathcal{E}_F(\rho_0) = \max \mathcal{E}_N = \min \mathcal{E}_{N+1}$ for some $N \geq 1$ (see (1.13)). This remains as a challenging open problem.

1.3. The Content of the Paper

Let us briefly discuss the content of the rest of this paper:

- In Sect. 2 we thoroughly analyze the behavior of the chemical potential μ_∞ when the temperature goes to zero defining the Fermi energy. These results are important for our main theorem.
- In Sect. 3 we give the most important technical result. Applying the magnetic perturbation theory we arrive at a general formula for $\mathcal{X}(\beta, \rho_0)$ which contains no derivatives with respect to $\mathbf{k}$. The strategy is somehow similar to the one used in [14] for the Faraday effect.

- In Sect. 4 we perform the zero temperature limit and separately analyze the situations in which the Fermi energy is either in an open spectral gap or inside the spectrum. It contains the proofs of Theorem 1.2 (i) and (ii).
- In Sect. 5 we obtain the Landau-Peierls formula by taking the low density limit. It contains the proof of Theorem 1.2 (iii).

2. The Fermi Energy

This section, which can be read independently of the rest of the paper, is only concerned with the location of the Fermi energy when the intensity of the magnetic field is zero (i.e. $\omega = 0$). In particular, we prove Theorem 1.1. Although we assumed in the introduction that $V \in \mathcal{C}^\infty(\mathbb{T}^3)$, all results of this section can be extended to the case $V \in L^\infty(\mathbb{T}^3)$.

2.1. Some Preparatory Results

Let $\xi \mapsto \mathfrak{f}(\beta,\mu;\xi) := \ln\left(1+\mathrm{e}^{\beta(\mu-\xi)}\right)$ be a holomorphic function on the domain $\{\xi \in \mathbb{C} : \Im\xi \in (-\pi/\beta, \pi/\beta)\}$. Let Γ the positively oriented simple contour included in the above domain defined by:

$$\Gamma := \left\{\Re\xi \in [\delta,\infty),\, \Im\xi = \pm\frac{\pi}{2\beta}\right\} \cup \left\{\Re\xi = \delta,\, \Im\xi \in \left[-\frac{\pi}{2\beta}, \frac{\pi}{2\beta}\right]\right\}, \quad (2.1)$$

where δ is any real number smaller than $E_0 := \inf\sigma(H_\infty(0)) \le \inf\sigma(H_\infty(\omega))$. In the following we use $\delta := E_0 - 1$.

The thermodynamic limit of the grand-canonical density at $\beta > 0, \mu \in \mathbb{R}$ and $\omega \ge 0$ is given by (see e.g. [8]):

$$\rho_\infty(\beta, \mathrm{e}^{\beta\mu}, \omega) = \frac{1}{|\Omega|}\frac{i}{2\pi}\mathrm{Tr}_{L^2(\mathbb{R}^3)}\left\{\chi_\Omega \int_\Gamma \mathrm{d}\xi\, \mathfrak{f}_{FD}(\beta,\mu;\xi)(H_\infty(\omega)-\xi)^{-1}\right\} \quad (2.2)$$

where $\mathfrak{f}_{FD}(\beta,\mu;\xi) := -\beta^{-1}\partial_\xi\mathfrak{f}(\beta,\mu;\xi) = (\mathrm{e}^{\beta(\xi-\mu)}+1)^{-1}$ is the Fermi-Dirac distribution function and χ_Ω denotes the characteristic function of Ω. We prove in [39] (even for singular potentials) that $\rho_\infty(\beta,\cdot,\omega)$ can be analytically extended to the domain $\mathbb{C} \setminus (-\infty, -\mathrm{e}^{\beta E_0(\omega)}]$.

Now assume that the intensity of the magnetic field is zero ($\omega = 0$). The following proposition (stated without proof since the result is well known), allows us to rewrite (2.2) only using the Bloch energy functions $\mathbf{k} \mapsto E_j(\mathbf{k})$ of $H_\infty(0)$:

Proposition 2.1. *Let $\beta > 0$ and $\mu \in \mathbb{R}$. Denote by Ω^* the first Brillouin zone of the dual lattice $2\pi\mathbb{Z}^3$. Then*:

$$\rho_\infty(\beta, \mathrm{e}^{\beta\mu}, 0) = \frac{1}{(2\pi)^3}\sum_{j=1}^{\infty}\int_{\Omega^*}\mathrm{d}\mathbf{k}\, \mathfrak{f}_{FD}(\beta,\mu;E_j(\mathbf{k})). \quad (2.3)$$

Note that another useful way to express the grand-canonical density at zero magnetic field consists in bringing into play the integrated density of states (IDS) of the operator $H_\infty(0)$ (see (1.10) for its definition):

$$\rho_\infty(\beta, \mathrm{e}^{\beta\mu}, 0) = -\int_{-\infty}^{\infty} \mathrm{d}\lambda\, \frac{\partial \mathfrak{f}_{FD}}{\partial \lambda}(\beta, \mu; \lambda) n_\infty(\lambda). \tag{2.4}$$

When the density of particles $\rho_0 > 0$ becomes the fixed parameter, the relation between the fugacity and density can be inverted. This is possible since for all $\beta > 0$, the map $\rho_\infty(\beta, \cdot, 0)$ is strictly increasing on $(0, \infty)$ and defines a $\mathcal{C}^\infty$-diffeomorphism of this interval onto itself. Then there exists an unique $z_\infty(\beta, \rho_0) \in (0, \infty)$ and therefore an unique $\mu_\infty(\beta, \rho_0) \in \mathbb{R}$ satisfying:

$$\rho_\infty(\beta, \mathrm{e}^{\beta\mu_\infty(\beta,\rho_0)}, 0) = \rho_0. \tag{2.5}$$

We now are interested in the zero temperature limit. The following proposition (again stated without proof) is a well known, straightforward consequence of the continuity of $n_\infty(\cdot)$:

Proposition 2.2. *Let $\mu \geq E_0 := \inf \sigma(H_\infty(0))$ be fixed. We have the identity*:

$$\lim_{\beta \to \infty} \rho_\infty(\beta, \mathrm{e}^{\beta\mu}, 0) = \frac{1}{(2\pi)^3} \sum_{j=1}^{\infty} \int_{\Omega^*} \mathrm{d}\mathbf{k}\, \chi_{[E_0,\mu]}(E_j(\mathbf{k})) = n_\infty(\mu), \tag{2.6}$$

where $\chi_{[E_0,\mu]}(\cdot)$ denotes the characteristic function of the interval $[E_0, \mu]$.

We end this paragraph with another preparatory result concerning the behavior of n_∞ near the edges of a spectral gap. This result is contained in the following lemma:

Lemma 2.3. *Let $\rho_0 > 0$ be fixed. Assume that there exists $N \geq 1$ such that $n_\infty(E) = \rho_0$ for all E satisfying $\max \mathcal{E}_N \leq E \leq \min \mathcal{E}_{N+1}$. We set $a_N := \max \mathcal{E}_N$ and $b_N := \min \mathcal{E}_{N+1}$. Assume that the gap is open, i.e. $a_N < b_N$. Then for $\delta > 0$ sufficiently small, there exists a constant $C = C_\delta > 0$ such that:*

$$n_\infty(a_N) - n_\infty(\lambda) \geq C(a_N - \lambda)^3 \quad \textit{whenever}\ \lambda \in [a_N - \delta, a_N] \tag{2.7}$$

and

$$n_\infty(\lambda) - n_\infty(b_N) \geq C(\lambda - b_N)^3 \quad \textit{whenever}\ \lambda \in [b_N, b_N + \delta]. \tag{2.8}$$

Proof. We only prove (2.7), since the proof of the other inequality (2.8) is similar. Since $a_N = \max_{\mathbf{k} \in \Omega^*} E_N(\mathbf{k})$, the maximum is attained in a (possibly not unique) point $\mathbf{k}_0$, i.e. $a_N = E_N(\mathbf{k}_0)$. This means that a_N is a discrete eigenvalue of finite multiplicity $1 \leq M \leq N$ of the fiber operator $h(\mathbf{k}_0) = \frac{1}{2}(-i\nabla + \mathbf{k}_0)^2 + V$. In particular, a_N is isolated from the rest of the spectrum since we assumed that $a_N < b_N \leq E_{N+1}(\mathbf{k}_0)$. Now when $\mathbf{k}$ slightly varies around $\mathbf{k}_0$, the eigenvalue a_N will split into at most M different eigenvalues, the largest of which being $E_N(\mathbf{k})$. Thus from the second equality in (2.6) we obtain:

$$n_\infty(a_N) - n_\infty(\lambda) \geq \frac{1}{(2\pi)^3} \mathrm{Vol}\{\mathbf{k} \in \Omega^* :\ \lambda \leq E_N(\mathbf{k}) \leq a_N\}.$$

We now choose δ small enough such that

$$\sigma(h(\mathbf{k}_0)) \cap [a_N - \delta, a_N + \delta] = \{E_N(\mathbf{k}_0)\}.$$

We use analytic perturbation theory in order to control the location of the spectrum of $h(\mathbf{k})$ when $|\mathbf{k} - \mathbf{k}_0|$ is small (we assume without loss of generality that $\mathbf{k}_0$ lies in the interior of Ω^*). By writing

$$h(\mathbf{k}) = h(\mathbf{k}_0) + (\mathbf{k} - \mathbf{k}_0) \cdot (-i\nabla + \mathbf{k}_0) + (\mathbf{k} - \mathbf{k}_0)^2/2 =: h(\mathbf{k}_0) + W(\mathbf{k}),$$

we see that we can find a constant $C > 0$ such that

$$\|W(\mathbf{k})(h(\mathbf{k}_0) - i)^{-1}\| \leq C|\mathbf{k} - \mathbf{k}_0|, \quad |\mathbf{k} - \mathbf{k}_0| \leq 1.$$

Take a circle γ with center at a_N and radius $r = (a_N - \lambda)/2 \leq \delta/2$. For any $z \in \gamma$, by virtue of the first resolvent equation:

$$(h(\mathbf{k}_0) - z)^{-1} = (h(\mathbf{k}_0) - i)^{-1} + (z - i)(h(\mathbf{k}_0) - i)^{-1}(h(\mathbf{k}_0) - z)^{-1}$$

and by using the estimate $\|(h(\mathbf{k}_0) - z)^{-1}\| = 2/(a_N - \lambda)$, we can find another constant $C_\delta > 0$ such that:

$$\sup_{z\in\gamma} \|W(\mathbf{k})(h(\mathbf{k}_0) - z)^{-1}\| \leq C_\delta \frac{|\mathbf{k} - \mathbf{k}_0|}{(a_N - \lambda)}, \quad |\mathbf{k} - \mathbf{k}_0| \leq 1.$$

It turns out that if $|\mathbf{k} - \mathbf{k}_0|/(a_N - \lambda)$ is smaller than some $\epsilon > 0$, then

$$\sup_{z\in\gamma} \|W(\mathbf{k})(h(\mathbf{k}_0) - z)^{-1}\| \leq \epsilon C_\delta \text{ whenever } |\mathbf{k} - \mathbf{k}_0| \leq (a_N - \lambda)\epsilon.$$

Standard analytic perturbation theory insures that if ϵ is chosen small enough, $h(\mathbf{k})$ will have exactly M eigenvalues inside γ. Thus for all $\mathbf{k}$ satisfying $|\mathbf{k}-\mathbf{k}_0| \leq \epsilon(a_N-\lambda)$, we have $\sigma(h(\mathbf{k}))\cap[a_N-\delta, a_N] \subseteq [(a_N+\lambda)/2, a_N] \subset [\lambda, a_N]$. In particular, $\lambda < E_N(\mathbf{k}) \leq a_N$ for all such $\mathbf{k}$'s. But the ball in Ω^* where $|\mathbf{k} - \mathbf{k}_0| \leq (a_N - \lambda)\epsilon$ has a volume which goes like $(a_N - \lambda)^3$, and the proof is finished. □

2.2. Proof of Theorem 1.1

In this paragraph we prove the existence of the Fermi energy. We separately investigate the semiconducting case and the metallic case.

2.2.1. The Semiconducting Case (SC). We here consider the same situation as in Lemma 2.3 in which there exists $N \geq 1$ such that $n_\infty(E) = \rho_0$ for all E satisfying $\max \mathcal{E}_N \leq E \leq \min \mathcal{E}_{N+1}$. We set $a_N := \max \mathcal{E}_N$ and $b_N := \min \mathcal{E}_{N+1}$. Let $\mu(\beta) := \mu_\infty(\beta, \rho_0)$ be the unique solution of the equation $\rho_\infty(\beta, \mathrm{e}^{\beta\mu}, 0) = \rho_0$. We start with the following lemma:

Lemma 2.4.

$$a_N \leq \mu_1 := \liminf_{\beta\to\infty} \mu(\beta) \leq \limsup_{\beta\to\infty} \mu(\beta) =: \mu_2 \leq b_N. \tag{2.9}$$

Proof. We will only prove the inequality $a_N \leq \mu_1$, since the proof of the other one ($\mu_2 \leq b_N$) is similar. Assume the contrary: $\mu_1 < a_N$. Define $\epsilon := a_N - \mu_1 > 0$.

Then there exists a sequence $\{\beta_n\}_{n\geq 1}$ with $\beta_n \to \infty$ and an integer $M_\epsilon \geq 1$ large enough such that:

$$\lim_{n\to\infty} \mu(\beta_n) = \mu_1 \quad \text{and} \quad \mu(\beta_n) \leq a_N - \epsilon/2 < a_N, \quad \forall n \geq M_\epsilon.$$

Since $\rho_\infty(\beta, \mathrm{e}^{\beta\mu}, 0)$ is an increasing function of μ, we have:

$$\rho_0 = \rho_\infty(\beta_n, \mathrm{e}^{\beta_n \mu(\beta_n)}, 0) \leq \rho_\infty(\beta_n, \mathrm{e}^{\beta_n(a_N - \epsilon/2)}, 0).$$

By letting $n \to \infty$ in the above inequality, (2.6) implies:

$$\rho_0 \leq n_\infty(a_N - \epsilon/2) < n_\infty(a_N) = \rho_0$$

where in the second inequality we used (2.7). We have arrived at a contradiction. □

Now if $a_N = b_N$, the proof of (1.13) is over. Thus we can assume that $a_N < b_N$, i.e. the gap is open. We have the following lemma:

Lemma 2.5. *Define $c_N = (a_N + b_N)/2$. For any $0 < \epsilon < (b_N - a_N)/2$, there exists $\beta_\epsilon > 0$ large enough such that $\mu(\beta) \in [c_N - \epsilon, c_N + \epsilon]$ whenever $\beta > \beta_\epsilon$.*

Proof. We know that $\mu(\beta)$ exists and is unique, thus if we can construct such a solution in the given interval, it means that this is the one. We use (2.4) in which we introduce $\mu(\beta)$ and arrive at the following identities:

$$\begin{aligned} n_\infty(a_N) &= \rho_0 \\ &= \int_{-\infty}^{\infty} \mathrm{d}\lambda \frac{\partial \mathfrak{f}_{FD}}{\partial \lambda}(\beta, \mu(\beta); \lambda) n_\infty(\lambda) = -\int_{-\infty}^{a_N} \mathrm{d}\lambda \frac{\partial \mathfrak{f}_{FD}}{\partial \lambda}(\beta, \mu(\beta); \lambda) n_\infty(\lambda) \\ &\quad - n_\infty(b_N)\mathfrak{f}_{FD}(\beta, \mu(\beta); b_N) + n_\infty(a_N)\mathfrak{f}_{FD}(\beta, \mu(\beta); a_N) \\ &\quad - \int_{b_N}^{\infty} \mathrm{d}\lambda \frac{\partial \mathfrak{f}_{FD}}{\partial \lambda}(\beta, \mu(\beta); \lambda) n_\infty(\lambda), \end{aligned}$$

where in the last term we used the fact that $n_\infty(\cdot)$ is constant on the interval $[a_N, b_N]$, and this constant is nothing but ρ_0. We can rewrite the above equation as:

$$\begin{aligned} &\int_{-\infty}^{a_N} \mathrm{d}\lambda \frac{\partial \mathfrak{f}_{FD}}{\partial \lambda}(\beta, \mu(\beta); \lambda)\{n_\infty(\lambda) - n_\infty(a_N)\} \\ &\quad = \int_{b_N}^{\infty} \mathrm{d}\lambda \frac{\partial \mathfrak{f}_{FD}}{\partial \lambda}(\beta, \mu(\beta); \lambda)\{n_\infty(b_N) - n_\infty(\lambda)\} \end{aligned} \tag{2.10}$$

where we used the fact that $\mathfrak{f}_{FD}(\beta, \mu(\beta); -\infty) = 1$ and $\mathfrak{f}_{FD}(\beta, \mu(\beta); \lambda) \leq C\mathrm{e}^{-\lambda\beta}$ for large λ.

In the left hand side of (2.10) we now introduce the explicit formula:

$$\partial_\lambda \mathfrak{f}_{FD}(\beta, \mu(\beta); \lambda) = -\beta \frac{\mathrm{e}^{\beta(\lambda - \mu(\beta))}}{(\mathrm{e}^{\beta(\lambda - \mu(\beta))} + 1)^2} = -\beta \mathrm{e}^{\beta(a_N - \mu(\beta))} \frac{\mathrm{e}^{\beta(\lambda - a_N)}}{(\mathrm{e}^{\beta(\lambda - \mu(\beta))} + 1)^2},$$

while in the right hand side of (2.10) we use another expression:

$$\partial_\lambda \mathfrak{f}_{FD}(\beta,\mu(\beta);\lambda) = -\beta\frac{\mathrm{e}^{-\beta(\lambda-\mu(\beta))}}{(1+\mathrm{e}^{-\beta(\lambda-\mu(\beta))})^2}$$
$$= -\beta\mathrm{e}^{-\beta(b_N-\mu(\beta))}\frac{\mathrm{e}^{-\beta(\lambda-b_N)}}{(1+\mathrm{e}^{-\beta(\lambda-\mu(\beta))})^2}.$$

Then (2.10) can be rewritten as:

$$\int_{-\infty}^{a_N} \mathrm{d}\lambda \frac{\mathrm{e}^{\beta(\lambda-a_N)}}{(\mathrm{e}^{\beta(\lambda-\mu(\beta))}+1)^2}\{n_\infty(a_N)-n_\infty(\lambda)\}$$
$$= \mathrm{e}^{\beta\{2\mu(\beta)-(a_N+b_N)\}}\int_{b_N}^{\infty} \mathrm{d}\lambda \frac{\mathrm{e}^{-\beta(\lambda-b_N)}}{(1+\mathrm{e}^{-\beta(\lambda-\mu(\beta))})^2}\{n_\infty(\lambda)-n_\infty(b_N)\}, \quad (2.11)$$

or by taking the logarithm:

$$\mu(\beta) = c_N + \frac{1}{2\beta}\left\{\ln\left(\int_{-\infty}^{a_N} \mathrm{d}\lambda \frac{\mathrm{e}^{\beta(\lambda-a_N)}}{(\mathrm{e}^{\beta(\lambda-\mu(\beta))}+1)^2}\{n_\infty(a_N)-n_\infty(\lambda)\}\right)\right.$$
$$\left. -\ln\left(\int_{b_N}^{\infty} \mathrm{d}\lambda \frac{\mathrm{e}^{-\beta(\lambda-b_N)}}{(1+\mathrm{e}^{-\beta(\lambda-\mu(\beta))})^2}\{n_\infty(\lambda)-n_\infty(b_N)\}\right)\right\}.$$

Let us define the smooth function $f:[c_N-\epsilon, c_N+\epsilon]\mapsto\mathbb{R}$ given by:

$$f(x) := c_N + \frac{1}{2\beta}\left\{\ln\left(\int_{-\infty}^{a_N} \mathrm{d}\lambda \frac{\mathrm{e}^{\beta(\lambda-a_N)}}{(\mathrm{e}^{\beta(\lambda-x)}+1)^2}\{n_\infty(a_N)-n_\infty(\lambda)\}\right)\right.$$
$$\left. -\ln\left(\int_{b_N}^{\infty} \mathrm{d}\lambda \frac{\mathrm{e}^{-\beta(\lambda-b_N)}}{(1+\mathrm{e}^{-\beta(\lambda-x)})^2}\{n_\infty(\lambda)-n_\infty(b_N)\}\right)\right\}. \quad (2.12)$$

We will prove that if β is large enough, then f invariates the interval $[c_N-\epsilon, c_N+\epsilon]$, which is already enough for the existence of a fixed point. This would also show that $\mu(\beta)$ must be in that interval. But in fact one can prove more: f is a contraction for large enough β.

The idea is to find some good upper and lower bounds when β is large for the integrals under the logarithms. We start by finding a lower bound in β for the first integral. Let $\delta>0$ sufficiently small. Using (2.7) in the left hand side of (2.11) we get:

$$\int_{-\infty}^{a_N} \mathrm{d}\lambda \frac{\mathrm{e}^{\beta(\lambda-a_N)}}{(\mathrm{e}^{\beta(\lambda-x)}+1)^2}\{n_\infty(a_N)-n_\infty(\lambda)\} \geq \frac{C}{4}\int_{a_N-\delta}^{a_N} \mathrm{e}^{-\beta(a_N-\lambda)}(a_N-\lambda)^3 \quad (2.13)$$

where we used that $x\geq a_N\geq\lambda$ in order to get rid of the numerator. After a change of variables and using some basic estimates one arrives at another constant $C > 0$ such that for β sufficiently large:

$$\int_{-\infty}^{a_N} \mathrm{d}\lambda \frac{\mathrm{e}^{\beta(\lambda - a_N)}}{(\mathrm{e}^{\beta(\lambda - x)} + 1)^2} \{n_\infty(a_N) - n_\infty(\lambda)\} \geq \frac{C}{\beta^5}. \tag{2.14}$$

By restricting the interval of integration to $[b_N, b_N + \delta]$ and by using (2.8), we obtain by the same method a similar lower bound for the second integral under the logarithm. Moreover, using the Weyl asymptotics which says that $n_\infty(\lambda) \sim \lambda^{\frac{3}{2}}$ for large λ (see e.g. [27]), one can also get a power-like upper bound in β for our two integrals.

We deduce from these estimates that there exists a constant $C_\epsilon > 0$ such that:

$$\sup_{x \in [c_N - \epsilon, c_N + \epsilon]} |f(x) - c_N| \leq \frac{C_\epsilon \ln(\beta)}{\beta}, \quad \beta > 1.$$

Thus if β is large enough, f invariates the interval. Being continuous, it must have a fixed point. Moreover, the derivative $f'(x)$ decays exponentially with β uniformly in $x \in [c_N - \epsilon, c_N + \epsilon]$. It implies that if β is large enough, then $\|f'\|_\infty < 1$, that is f is a contraction. □

2.2.2. The Metallic Case (M). Consider the situation in which there exists a unique solution E_M of the equation $n_\infty(E_M) = \rho_0$, and this solution lies in the interior of a Bloch band. In other words, there exists (a possibly not unique) integer $N \geq 1$ such that $\min \mathcal{E}_N < E_M < \max \mathcal{E}_N$. We will use in the following that the IDS $n_\infty(\cdot)$ is a strictly increasing function on the interval $[\min \mathcal{E}_N, \max \mathcal{E}_N]$.

Let $\mu(\beta) := \mu_\infty(\beta, \rho_0)$ be the unique real solution of the equation $\rho_\infty(\beta, \mathrm{e}^{\beta\mu(\beta)}, 0) = \rho_0$. Let us show that:

$$E_M \leq \liminf_{\beta \to \infty} \mu(\beta) \leq \limsup_{\beta \to \infty} \mu(\beta) \leq E_M, \tag{2.15}$$

which would end the proof. We start with the first inequality.

Assume ad-absurdum that $\mu_1 := \liminf_{\beta \to \infty} \mu(\beta) < E_M$. Then there exists $\epsilon > 0$ and a sequence $\{\beta_n\}_{n \geq 1}$ satisfying $\beta_n \to \infty$ such that:

$$\lim_{n \to \infty} \mu(\beta_n) = \mu_1, \quad \mu(\beta_n) \leq E_M - \epsilon, \quad \forall n \geq 1.$$

Since $\rho_\infty(\beta, \mathrm{e}^{\beta\mu}, 0)$ is increasing with μ, we have:

$$\begin{aligned} n_\infty(E_M) = \rho_0 &= \lim_{n \to \infty} \rho_\infty(\beta_n, \mathrm{e}^{\beta_n \mu(\beta_n)}, 0) \\ &\leq \lim_{n \to \infty} \rho_\infty(\beta_n, \mathrm{e}^{\beta_n(E_M - \epsilon)}, 0) = n_\infty(E_M - \epsilon), \end{aligned} \tag{2.16}$$

where in the last equality we used (2.6). But the inequality $n_\infty(E_M) \leq n_\infty(E_M - \epsilon)$ is in contradiction with the fact that $n_\infty(\cdot)$ is a strictly increasing function near E_M. Thus $E_M \leq \mu_1$.

Now assume ad-absurdum that $\mu_2 := \limsup_{\beta \to \infty} \mu(\beta) > E_M$. Then there exists $\epsilon > 0$ and a sequence $\{\beta_n\}_{n \geq 1}$ satisfying $\beta_n \to \infty$ such that:

$$\lim_{n \to \infty} \mu(\beta_n) = \mu_2, \quad E_M + \epsilon \leq \mu(\beta_n), \quad \forall n \geq 1.$$

We again use that $\rho_\infty(\beta, \mathrm{e}^{\beta\mu}, 0)$ is increasing with μ and write:

$$\begin{aligned} n_\infty(E_M+\epsilon) &= \lim_{n\to\infty} \rho_\infty(\beta_n, \mathrm{e}^{\beta_n(E_M+\epsilon)}, 0) \\ &\leq \lim_{n\to\infty} \rho_\infty(\beta_n, \mathrm{e}^{\beta_n\mu(\beta_n)}, 0) = \rho_0 = n_\infty(E_M), \end{aligned} \tag{2.17}$$

where in the first equality we again used (2.6). But the inequality $n_\infty(E_M+\epsilon) \leq n_\infty(E_M)$ is also in contradiction with the fact that $n_\infty(\cdot)$ is a strictly increasing function near E_M. Therefore $\mu_2 \leq E_M$. □

3. The Zero-Field Susceptibility at Fixed Density and Positive Temperature

In this section we prove a general formula for the zero-field grand-canonical susceptibility of a Bloch electrons gas at fixed density and positive temperature.

Here is the main result of this section:

Theorem 3.1. *Let $\beta > 0$ and $\rho_0 > 0$ be fixed. Let $\mu_\infty = \mu_\infty(\beta, \rho_0) \in \mathbb{R}$ the unique solution of the equation $\rho_\infty(\beta, \mathrm{e}^{\beta\mu}, \omega = 0) = \rho_0$. Then for each integer $j_1 \geq 1$ there exists four families of functions $\mathfrak{c}_{j_1,l}(\cdot)$, with $l \in \{0,1,2,3\}$, defined on Ω^* outside a set of Lebesgue measure zero, such that the integrand below can be extended by continuity to the whole of Ω^*:*

$$\mathcal{X}(\beta,\rho_0) = -\left(\frac{\mathrm{e}}{c}\right)^2 \frac{1}{2\beta}\frac{1}{(2\pi)^3}\sum_{j_1=1}^{\infty}\int_{\Omega^*}\mathrm{d}\mathbf{k}\sum_{l=0}^{3}\frac{\partial^l \mathfrak{f}}{\partial \xi^l}(\beta,\mu_\infty;E_{j_1}(\mathbf{k}))\,\mathfrak{c}_{j_1,l}(\mathbf{k}), \tag{3.1}$$

with the convention $(\partial_\xi^0 \mathfrak{f})(\beta,\mu_\infty;E_{j_1}(\mathbf{k})) = \mathfrak{f}(\beta,\mu_\infty;E_{j_1}(\mathbf{k})) := \ln(1 + \mathrm{e}^{\beta(\mu_\infty - E_{j_1}(\mathbf{k}))})$.

This formula is a necessary step in the proof of Theorem 1.2 (*i*) and (*ii*) (this is the aim of the following section) when we will take the limit of zero temperature.

The special feature of this formula lies in the fact that each function $\mathfrak{c}_{j_1,l}(\cdot)$ can be only expressed in terms of Bloch energy functions and their associated eigenfunctions. For each integer $j_1 \geq 1$, the functions $\mathfrak{c}_{j_1,2}(\cdot)$ and $\mathfrak{c}_{j_1,3}(\cdot)$ are identified respectively in (3.28) and (3.27). As for the functions $\mathfrak{c}_{j_1,l}(\cdot)$ with $l \in \{0,1\}$, they can also be written down but their explicit expression is not important for the proof of Theorem 1.2. Note as well that the above formula brings into play the Fermi–Dirac distribution and its partial derivatives up to the second order. This will turn out to be very important when we will take the limit $\beta \to \infty$ in the following section.

3.1. Starting the Proof: A General Formula from the Magnetic Perturbation Theory

We start by giving a useful formula for the thermodynamic limit of the grand-canonical susceptibility. Let $\beta > 0$ and $z := \mathrm{e}^{\beta\mu} \in (0,\infty)$ the fixed external parameters. Let Γ be the positively oriented contour defined in (2.1), going round the half-line $[E_0,\infty)$, and included in the analiticity domain of the map $\xi \mapsto \mathfrak{f}(\beta,z;\xi) = \ln(1+z\mathrm{e}^{-\beta\xi})$. Denote by $R_\infty(\omega,\xi) := (H_\infty(\omega)-\xi)^{-1}$ for all $\xi \in \rho(H_\infty(\omega))$ and $\omega \in \mathbb{R}$. Taking into account the periodic structure of our system, it is proved (see [7], Theorem 3.8) that the thermodynamic limit of the grand-canonical pressure of the Bloch electron gas at any intensity of the magnetic field B is given by:

$$P_\infty(\beta,z,\omega) := \frac{1}{\beta|\Omega|}\frac{i}{2\pi}\mathrm{Tr}_{L^2(\mathbb{R}^3)}\left\{\chi_\Omega \int_\Gamma \mathrm{d}\xi\, \mathfrak{f}(\beta,z;\xi)R_\infty(\omega,\xi)\right\}, \tag{3.2}$$

where Ω is the unit cube centered at the origin of coordinates (χ_Ω denotes its characteristic function). Although the integral kernel $R_\infty(\cdot\,,\cdot\,;\omega,\xi)$ of the resolvent has a singularity on the diagonal, the integration with respect to ξ in (3.2) provides us with a jointly continuous kernel on $\mathbb{R}^3\times\mathbb{R}^3$. One can see this by performing an integration by parts in (3.2) and using the fact that the kernel of $R^2_\infty(\omega,\xi)$ is jointly continuous. Moreover, one can prove [4–6] that the thermodynamic limit of the grand-canonical pressure is jointly smooth on $(z,\omega) \in (-\mathrm{e}^{\beta E_0},\infty)\times\mathbb{R}$.

Let $\omega \in \mathbb{R}$ and $\xi \in \rho(H_\infty(\omega))$. Introduce the bounded operators $T_{\infty,1}(\omega,\xi)$ and $T_{\infty,2}(\omega,\xi)$ generated by the following integral kernels:

$$T_{\infty,1}(\mathbf{x},\mathbf{y};\omega,\xi) := \mathbf{a}(\mathbf{x}-\mathbf{y})\cdot(i\nabla_\mathbf{x}+\omega\mathbf{a}(\mathbf{x}))R_\infty(\mathbf{x},\mathbf{y};\omega,\xi) \tag{3.3}$$

$$T_{\infty,2}(\mathbf{x},\mathbf{y};\omega,\xi) := \frac{1}{2}\mathbf{a}^2(\mathbf{x}-\mathbf{y})R_\infty(\mathbf{x},\mathbf{y};\omega,\xi), \quad \mathbf{x}\neq\mathbf{y}, \tag{3.4}$$

where $\mathbf{a}(\cdot)$ stands for the usual symmetric gauge $\mathbf{a}(\mathbf{x}) = \frac{1}{2}\mathbf{e}_3\wedge\mathbf{x} = \frac{1}{2}(-x_2,x_1,0)$. We introduce the following operators :

$$\mathcal{W}_{\infty,1}(\beta,\mu,\omega) := \frac{i}{2\pi}\int_\Gamma \mathrm{d}\xi\, \mathfrak{f}(\beta,\mu;\xi)R_\infty(\omega,\xi)T_{\infty,1}(\omega,\xi)T_{\infty,1}(\omega,\xi) \tag{3.5}$$

$$\mathcal{W}_{\infty,2}(\beta,\mu,\omega) := \frac{i}{2\pi}\int_\Gamma \mathrm{d}\xi\, \mathfrak{f}(\beta,\mu;\xi)R_\infty(\omega,\xi)T_{\infty,2}(\omega,\xi) \tag{3.6}$$

One can prove using the same techniques as in [15] that these operators are locally trace class and have a jointly continuous kernel on $\mathbb{R}^3\times\mathbb{R}^3$. By a closely related method as the one in [4,5], it is proved in [39] that we can invert the thermodynamic limit with the partial derivatives w.r.t. ω of the grand-canonical pressure. Then the bulk orbital susceptibility reads as:

$$\begin{aligned}\mathcal{X}^{GC}_\infty(\beta,\mathrm{e}^{\beta\mu},\omega) &:= \left(\frac{\mathrm{e}}{c}\right)^2\frac{\partial^2 P_\infty}{\partial\omega^2}(\beta,\mathrm{e}^{\beta\mu},\omega)\\ &= \left(\frac{\mathrm{e}}{c}\right)^2\frac{2}{\beta|\Omega|}\left\{\mathrm{Tr}_{L^2(\mathbb{R}^3)}\left\{\chi_\Omega\mathcal{W}_{\infty,1}(\beta,\mu,\omega)\right\}\right.\\ &\qquad\left.-\mathrm{Tr}_{L^2(\mathbb{R}^3)}\left\{\chi_\Omega\mathcal{W}_{\infty,2}(\beta,\mu,\omega)\right\}\right\}\end{aligned}$$

We mention that the above formula is obtained using the so-called 'gauge invariant magnetic perturbation theory' applied to the resolvent integral kernel (see e.g. [15] for further details) which allows to control the linear growth of the magnetic vector potential.

The quantity which we are interested in is the orbital susceptibility at zero magnetic field and at fixed density of particles ρ_0. Note that the pressure is an even function of ω, thus its first order derivative at $\omega = 0$ is zero. This explains why the susceptibility is the relevant physical quantity for the weak magnetic field regime.

The orbital susceptibility at zero magnetic field and fixed density ρ_0 is given by (see also (1.8)):

$$\begin{aligned}\mathcal{X}(\beta, \rho_0) :&= \mathcal{X}_\infty^{GC}(\beta, \mathrm{e}^{\beta\mu_\infty(\beta,\rho_0)}, 0)\\ &= \left(\frac{\mathrm{e}}{c}\right)^2 \frac{2}{\beta|\Omega|} \left\{\mathrm{Tr}_{L^2(\mathbb{R}^3)} \left\{\chi_\Omega \mathcal{W}_{\infty,1}(\beta, \mu_\infty, 0)\right\}\right.\\ &\qquad \left. - \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left\{\chi_\Omega \mathcal{W}_{\infty,2}(\beta, \mu_\infty, 0)\right\}\right\}. \end{aligned} \tag{3.7}$$

The formula (3.7) constitutes the starting-point in obtaining (3.1). The next step consists in rewriting the local traces appearing in (3.7) in a more convenient way:

Proposition 3.2. *Let* $p_\alpha := -i\partial_\alpha$ *with* $\alpha \in \{1, 2, 3\}$ *be the cartesian components of the momentum operator defined in* $L^2(\mathbb{R}^3)$. *Then we have*:

$$\begin{aligned}&\mathrm{Tr}_{L^2(\mathbb{R}^3)} \left\{\chi_\Omega \mathcal{W}_{\infty,1}(\beta, \mu_\infty, 0)\right\}\\ &= \frac{1}{4}\frac{i}{2\pi} \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left\{ \chi_\Omega \int_\Gamma \mathrm{d}\xi\, \mathfrak{f}(\beta, \mu_\infty; \xi) \left[R_\infty(0,\xi) p_1 R_\infty(0,\xi) p_2 R_\infty(0,\xi)\right.\right.\\ &\quad \times \left\{p_2 R_\infty(0,\xi) p_1 R_\infty(0,\xi) - p_1 R_\infty(0,\xi) p_2 R_\infty(0,\xi)\right\}\\ &\quad + R_\infty(0,\xi) p_2 R_\infty(0,\xi) p_1 R_\infty(0,\xi)\\ &\quad \left.\left. \times \left\{p_1 R_\infty(0,\xi) p_2 R_\infty(0,\xi) - p_2 R_\infty(0,\xi) p_1 R_\infty(0,\xi)\right\}\right]\right\} \end{aligned} \tag{3.8}$$

and

$$\begin{aligned}\mathrm{Tr}_{L^2(\mathbb{R}^3)} \left\{\chi_\Omega \mathcal{W}_{\infty,2}(\beta, \mu_\infty, 0)\right\} &= -\frac{1}{4}\frac{i}{2\pi} \mathrm{Tr}_{L^2(\mathbb{R}^3)} \left\{ \chi_\Omega \int_\Gamma \mathrm{d}\xi\, \mathfrak{f}(\beta, \mu_\infty; \xi)\right.\\ &\quad \times R_\infty(0,\xi) R_\infty(0,\xi) \left[p_2 R_\infty(0,\xi) p_2 R_\infty(0,\xi)\right.\\ &\quad \left.\left. + p_1 R_\infty(0,\xi) p_1 R_\infty(0,\xi) - R_\infty(0,\xi)\right]\right\}. \end{aligned} \tag{3.9}$$

Proof. We begin with the justification of (3.9). By rewriting (3.4) as:

$$T_{\infty,2}(\mathbf{x},\mathbf{y};0,\xi) = \frac{1}{8}\{\mathbf{e}_3 \wedge (\mathbf{x}-\mathbf{y})\}\cdot\{\mathbf{e}_3 \wedge (\mathbf{x}-\mathbf{y})\}R_\infty(\mathbf{x},\mathbf{y};0,\xi)$$
$$= \frac{1}{8}\left[(x_2-y_2)^2 + (x_1-y_1)^2\right] R_\infty(\mathbf{x},\mathbf{y};0,\xi),$$

from (3.6) it follows:

$$\mathcal{W}_{\infty,2}(\mathbf{x},\mathbf{x};\beta,\mu,0) = \frac{1}{8}\int_\Gamma \mathrm{d}\xi\, \mathfrak{f}(\beta,\mu;\xi)\int_{\mathbb{R}^3}\mathrm{d}\mathbf{z}\, R_\infty(\mathbf{x},\mathbf{z};0,\xi)\left[(z_2-x_2)^2\right.$$
$$\left.+(z_1-x_1)^2\right] R_\infty(\mathbf{z},\mathbf{x};0,\xi), \quad \forall\, \mathbf{x}\in\mathbb{R}^3. \tag{3.10}$$

Let $l \in \{1,2\}$. Denote by $\mathbf{X}$ the multiplication operator with $\mathbf{x}$. Then for all $\mathbf{z}\neq\mathbf{x}$ we can write:

$$(z_l - x_l)R_\infty(\mathbf{z},\mathbf{x};0,\xi) = [\mathbf{X}\cdot\mathbf{e}_l, R_\infty(0,\xi)]\,(\mathbf{z},\mathbf{x})$$
$$= \{R_\infty(0,\xi)\,[H_\infty(0),\mathbf{X}\cdot\mathbf{e}_l]\,R_\infty(0,\xi)\}\,(\mathbf{z},\mathbf{x}).$$

We know that $[H_\infty(0),\mathbf{X}\cdot\mathbf{e}_l] = -ip_l$. Thus:

$$(z_l - x_l)R_\infty(\mathbf{z},\mathbf{x};0,\xi) = -i\,\{R_\infty(0,\xi)p_l R_\infty(0,\xi)\}\,(\mathbf{z},\mathbf{x}). \tag{3.11}$$

Using standard commutation rules, we deduce from (3.11) that for $l\in\{1,2\}$ and for all $\mathbf{z}\neq\mathbf{x}$:

$$(z_l - x_l)^2 R_\infty(\mathbf{z},\mathbf{x};0,\xi)$$
$$= -\{2R_\infty(0,\xi)p_l R_\infty(0,\xi)p_l R_\infty(0,\xi) - R_\infty(0,\xi)R_\infty(0,\xi)\}\,(\mathbf{z},\mathbf{x}). \tag{3.12}$$

It remains to put (3.12) in (3.10), and we get (3.9).

Let us now prove now (3.8). Since the divergence of $\mathbf{a}$ is zero, then for $\mathbf{x}\neq\mathbf{y}$ we have:

$$T_{\infty,1}(\mathbf{x},\mathbf{y};0,\xi) = \frac{i}{2}\nabla_{\mathbf{x}}\cdot\{\mathbf{e}_3\wedge(\mathbf{x}-\mathbf{y})\}R_\infty(\mathbf{x},\mathbf{y};0,\xi)$$
$$= i\nabla_{\mathbf{x}}\cdot\left[-\frac{(x_2-y_2)}{2}\mathbf{e}_1 + \frac{(x_1-y_1)}{2}\mathbf{e}_2\right]R_\infty(\mathbf{x},\mathbf{y};0,\xi).$$

From (3.5) it follows that for all $\mathbf{x}\in\mathbb{R}^3$:

$$\mathcal{W}_{\infty,1}(\mathbf{x},\mathbf{x};\beta,\mu,0) = \frac{1}{4}\int_\Gamma \mathrm{d}\xi\,\mathfrak{f}(\beta,\mu;\xi)\int_{\mathbb{R}^3}\mathrm{d}\mathbf{z}_1\int_{\mathbb{R}^3}\mathrm{d}\mathbf{z}_2\, R_\infty(\mathbf{x},\mathbf{z}_1;0,\xi)$$
$$\times\{(i\nabla_{\mathbf{z}_1}\cdot\mathbf{e}_1)[-(z_{1,2}-z_{2,2})R_\infty(0,\xi)(\mathbf{z}_1,\mathbf{z}_2)]$$
$$+(i\nabla_{\mathbf{z}_1}\cdot\mathbf{e}_2)[(z_{1,1}-z_{2,1})R_\infty(0,\xi)(\mathbf{z}_1,\mathbf{z}_2)]\}$$
$$\cdot\{(i\nabla_{\mathbf{z}_2}\cdot\mathbf{e}_1)[-(z_{2,2}-x_2)R_\infty(0,\xi)(\mathbf{z}_2,\mathbf{x})]$$
$$+(i\nabla_{\mathbf{z}_2}\cdot\mathbf{e}_2)[(z_{2,1}-x_1)R_\infty(0,\xi)(\mathbf{z}_2,\mathbf{x})]\}.$$

Then by using (3.11), we get (3.8) from the following identity:

$$\begin{aligned}
&\forall\, \mathbf{x} \in \mathbb{R}^3, \quad \mathcal{W}_{\infty,1}(\mathbf{x},\mathbf{x};\beta,\mu,0)\\
&= \frac{1}{4}\int_{\Gamma} \mathrm{d}\xi\, \mathfrak{f}(\beta,\mu;\xi) \int_{\mathbb{R}^3} \mathrm{d}\mathbf{z}_1 \int_{\mathbb{R}^3} \mathrm{d}\mathbf{z}_2\, R_\infty(\mathbf{x},\mathbf{z}_1;0,\xi)\\
&\{ip_1\left(R_\infty(0,\xi)p_2R_\infty(0,\xi)\right)(\mathbf{z}_1,\mathbf{z}_2) - ip_2\left(R_\infty(0,\xi)p_1R_\infty(0,\xi)\right)(\mathbf{z}_1,\mathbf{z}_2)\}\\
&\{ip_1\left(R_\infty(0,\xi)p_2R_\infty(0,\xi)\right)(\mathbf{z}_2,\mathbf{x}) - ip_2\left(R_\infty(0,\xi)p_1R_\infty(0,\xi)\right)(\mathbf{z}_2,\mathbf{x})\}.
\end{aligned}$$

□

3.2. Using the Bloch Decomposition

We know that (see e.g. [10]) $H_\infty(0)$ can be seen as a direct integral $\int_{\Omega^*}^{\oplus} \mathrm{d}\mathbf{k}\, h(\mathbf{k})$ where the fiber Hamiltonians $h(\mathbf{k})$ acting in $L^2(\mathbb{T}^3)$ are given by:

$$h(\mathbf{k}) = \frac{1}{2}(-i\nabla + \mathbf{k})^2 + V. \tag{3.13}$$

Recall that $h(\mathbf{k})$ is essentially self-adjoint in $\mathcal{C}^\infty(\mathbb{T}^3)$; the domain of its closure is the Sobolev space $\mathcal{H}^2(\mathbb{T}^3)$. For each $\mathbf{k} \in \Omega^*, h(\mathbf{k})$ has purely discrete spectrum. We have already denoted by $\{E_j(\mathbf{k})\}_{j\geq 1}$ the set of eigenvalues counting multiplicities and in increasing order. The corresponding eigenfunctions $\{u_j(\cdot\,;\mathbf{k})\}_{j\geq 1}$ form a complete orthonormal system in $L^2(\mathbb{T}^3)$ and satisfy:

$$h(\mathbf{k})u_j(\cdot;\mathbf{k}) = E_j(\mathbf{k})u_j(\cdot;\mathbf{k}).$$

The eigenfunctions u_j's are defined up to an arbitrary phase depending on $\mathbf{k}$. These phases cannot be always chosen to be continuous at crossing points, and even less differentiable. For the following let us introduce another notation. Let $\alpha \in \{1,2,3\}$, and let $i, j \geq 1$ be any natural numbers. Then for all $\mathbf{k} \in \Omega^*$ we define:

$$\hat{\pi}_{i,j}(\alpha;\mathbf{k}) := \int_{\Omega} \mathrm{d}\mathbf{x}\, \overline{u_i(\mathbf{x};\mathbf{k})}[(p_\alpha + k_\alpha)u_j(\mathbf{x};\mathbf{k})] = \langle u_i(\cdot\,;\mathbf{k}), (p_\alpha + k_\alpha)u_j(\cdot\,;\mathbf{k})\rangle. \tag{3.14}$$

Note that due to the phases presence in the eigenfunctions u_j's, we cannot be sure that the $\hat{\pi}_{i,j}$'s are continuous/differentiable at crossing points. But all these 'bad' phase factors will disappear when we take the traces (see (3.20) and (3.23) below).

We now can write the local traces of Proposition 3.2 in the following way:

Proposition 3.3. *Let $\beta > 0$ and $\rho_0 > 0$ be fixed. Let $\mu_\infty = \mu_\infty(\beta,\rho_0) \in \mathbb{R}$ be the unique solution of the equation $\rho_\infty(\beta, \mathrm{e}^{\beta\mu}, 0) = \rho_0$. Then both quantities* (3.8) *and* (3.9) *can be rewritten as*:

$$\begin{aligned}
\mathrm{Tr}_{L^2(\mathbb{R}^3)}\left\{\chi_\Omega \mathcal{W}_{\infty,1}(\beta,\mu_\infty,0)\right\} &= -\frac{1}{4}\frac{1}{|\Omega^*|}\sum_{j_1,\dots,j_4=1}^{\infty}\int_{\Omega^*}\mathrm{d}\mathbf{k}\,\mathcal{C}_{j_1,j_2,j_3,j_4}(\mathbf{k})\\
&\times \frac{1}{2i\pi}\int_\Gamma \mathrm{d}\xi\, \frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{\left(E_{j_1}(\mathbf{k})-\xi\right)^2\left(E_{j_2}(\mathbf{k})-\xi\right)\left(E_{j_3}(\mathbf{k})-\xi\right)\left(E_{j_4}(\mathbf{k})-\xi\right)},
\end{aligned} \tag{3.15}$$

and

$$\begin{aligned}&\mathrm{Tr}_{L^2(\mathbb{R}^3)}\left\{\chi_\Omega \mathcal{W}_{\infty,2}(\beta,\mu_\infty,0)\right\}\\&= -\frac{1}{4}\frac{1}{|\Omega^*|}\left\{\sum_{j_1=1}^{\infty}\int_{\Omega^*}\mathrm{d}\mathbf{k}\,\frac{1}{2i\pi}\int_\Gamma \mathrm{d}\xi\,\frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{(E_{j_1}(\mathbf{k})-\xi)^3}+\right.\\&\quad\left.-\sum_{j_1,j_2=1}^{\infty}\int_{\Omega^*}\mathrm{d}\mathbf{k}\,\mathcal{C}_{j_1,j_2}(\mathbf{k})\frac{1}{2i\pi}\int_\Gamma \mathrm{d}\xi\,\frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{(E_{j_1}(\mathbf{k})-\xi)^3(E_{j_2}(\mathbf{k})-\xi)}\right\},\end{aligned}\tag{3.16}$$

where the functions $\Omega^* \ni \mathbf{k} \mapsto \mathcal{C}_{j_1,j_2,j_3,j_4}(\mathbf{k})$ *and* $\Omega^* \ni \mathbf{k} \mapsto \mathcal{C}_{j_1,j_2}(\mathbf{k})$ *are defined by*:

$$\begin{aligned}\mathcal{C}_{j_1,j_2,j_3,j_4}(\mathbf{k}) :=& \left\{\hat{\pi}_{j_1,j_2}(1;\mathbf{k})\hat{\pi}_{j_2,j_3}(2;\mathbf{k}) - \hat{\pi}_{j_1,j_2}(2;\mathbf{k})\hat{\pi}_{j_2,j_3}(1;\mathbf{k})\right\}\\&\times\left\{\hat{\pi}_{j_3,j_4}(2;\mathbf{k})\hat{\pi}_{j_4,j_1}(1;\mathbf{k}) - \hat{\pi}_{j_3,j_4}(1;\mathbf{k})\hat{\pi}_{j_4,j_1}(2;\mathbf{k})\right\}\end{aligned}\tag{3.17}$$

and

$$\begin{aligned}\mathcal{C}_{j_1,j_2}(\mathbf{k}) &:= \hat{\pi}_{j_1,j_2}(1;\mathbf{k})\hat{\pi}_{j_2,j_1}(1;\mathbf{k}) + \hat{\pi}_{j_1,j_2}(2;\mathbf{k})\hat{\pi}_{j_2,j_1}(2;\mathbf{k})\\&= \left|\hat{\pi}_{j_1,j_2}(1;\mathbf{k})\right|^2 + \left|\hat{\pi}_{j_1,j_2}(2;\mathbf{k})\right|^2.\end{aligned}\tag{3.18}$$

We do not give more details since this result is just a straightforward application of the following rather non-trivial technical lemma (recently proved in [16]):

Lemma 3.4. *Let* $\beta > 0$ *and* $\mu \in \mathbb{R}$ *be fixed. For* $n, m \in \mathbb{N}$ *with* $m, n \geq 1$, *consider the local trace given by*:

$$\begin{aligned}\mathcal{J}^{(m)}_{\alpha_1,\ldots,\alpha_n} := \mathrm{Tr}_{L^2(\mathbb{R}^3)}&\left\{\chi_\Omega \int_\Gamma \mathrm{d}\xi\,\mathfrak{f}(\beta,\mu;\xi)(H_\infty(0)-\xi)^{-m}p_{\alpha_1}\right.\\&\left.\times(H_\infty(0)-\xi)^{-1}\cdots p_{\alpha_n}(H_\infty(0)-\xi)^{-1}\right\}\end{aligned}$$

Then under the assumption that $V \in \mathcal{C}^\infty(\mathbb{T}^3)$ *we have*:

$$\begin{aligned}\mathcal{J}^{(m)}_{\alpha_1,\ldots,\alpha_n} =& \frac{1}{|\Omega^*|}\sum_{j_1,\ldots,j_n\geq 1}\int_{\Omega^*}\mathrm{d}\mathbf{k}\,\hat{\pi}_{j_1,j_2}(\alpha_1;\mathbf{k})\ldots\hat{\pi}_{j_n,j_1}(\alpha_n;\mathbf{k})\\&\times\int_\Gamma \mathrm{d}\xi\,\frac{\mathfrak{f}(\beta,\mu;\xi)}{(E_{j_1}(\mathbf{k})-\xi)^{m+1}(E_{j_2}(\mathbf{k})-\xi)\cdots(E_{j_n}(\mathbf{k})-\xi)}.\end{aligned}\tag{3.19}$$

where all the above series are absolutely convergent and $\hat{\pi}_{i,j}(\alpha;\mathbf{k})$ *is defined by* (3.14).

3.3. Applying the Residue Calculus

Consider the expression of the susceptibility at fixed density (3.7) in which the local traces are now given by (3.15) and (3.16). Remark that these quantities now are written in a convenient way in order to apply the residue theorem. Denote the integrands appearing in (3.15) and (3.16) by:

$$\mathfrak{g}_{j_1,j_2}(\beta,\mu_\infty;\xi) := \frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{\left(E_{j_1}(\mathbf{k})-\xi\right)^3\left(E_{j_2}(\mathbf{k})-\xi\right)}, \quad j_1,j_2\in\mathbb{N}^*$$

$$\mathfrak{h}_{j_1,j_2,j_3,j_4}(\beta,\mu_\infty;\xi) := \frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{\left(E_{j_1}(\mathbf{k})-\xi\right)^2\left(E_{j_2}(\mathbf{k})-\xi\right)\left(E_{j_3}(\mathbf{k})-\xi\right)\left(E_{j_4}(\mathbf{k})-\xi\right)}, \quad j_1,j_2,j_3,j_4\in\mathbb{N}^*.$$

Note that $\mathfrak{g}_{j_1,j_2}(\beta,\mu_\infty;\cdot)$ can have first order, third order, or even fourth order poles (in the case when $j_1=j_2$). In the same way, $\mathfrak{h}_{j_1,j_2,j_3,j_4}(\beta,\mu_\infty;\cdot)$ can have poles from the first order up to at most fifth order (in the case when $j_1=j_2=j_3=j_4$). Hence we expect that the integrals of $\mathfrak{h}_{j_1,j_2,j_3,j_4}(\beta,\mu_\infty;\cdot)$ in (3.15) (resp. of $\mathfrak{g}_{j_1,j_2}(\beta,\mu_\infty;\cdot)$ in (3.16)) to make appear partial derivatives of $\mathfrak{f}(\beta,\mu_\infty;\cdot)$ with order at most 4 (resp. with order at most 3). But we will see below that the factor multiplying $(\partial_\xi^4\mathfrak{f})(\beta,\mu_\infty;\cdot)$ is identically zero.

Getting back to the susceptibility formula in (3.7) and by virtue of the previous remarks, we expect to obtain an expansion of the orbital susceptibility of the type (3.1). The next two results identify the *functions* $\mathfrak{c}_{j_1,l}(\cdot)$ coming from (3.15) and (3.16):

Lemma 3.5. *The quantity defined by* (3.15) *can be rewritten as:*

$$\operatorname{Tr}_{L^2(\mathbb{R}^3)}\left\{\chi_\Omega\mathcal{W}_{\infty,1}(\beta,\mu_\infty)\right\} = -\frac{1}{4}\frac{1}{|\Omega^*|}\sum_{j_1=1}^{\infty}\int_{\Omega^*}\mathrm{d}\mathbf{k}\sum_{l=0}^{3}\frac{\partial^l\mathfrak{f}}{\partial\xi^l}\left(\beta,\mu_\infty;E_{j_1}(\mathbf{k})\right)\mathfrak{a}_{j_1,l}(\mathbf{k}) \tag{3.20}$$

where for all $j_1\in\mathbb{N}^*$ and $\mathbf{k}\in\Omega^*$, the functions $\mathfrak{a}_{j_1,3}(\cdot)$ and $\mathfrak{a}_{j_1,2}(\cdot)$ are given by:

$$\begin{aligned}\mathfrak{a}_{j_1,3}(\mathbf{k}) := \frac{1}{3!}\Bigg\{&\left|\hat{\pi}_{j_1,j_1}(1;\mathbf{k})\right|^2\sum_{\substack{j_2=1\\ j_2\neq j_1}}^{\infty}\frac{\left|\hat{\pi}_{j_1,j_2}(2;\mathbf{k})\right|^2}{E_{j_2}(\mathbf{k})-E_{j_1}(\mathbf{k})}\\ &+\left|\hat{\pi}_{j_1,j_1}(2;\mathbf{k})\right|^2\sum_{\substack{j_2=1\\ j_2\neq j_1}}^{\infty}\frac{\left|\hat{\pi}_{j_1,j_2}(1;\mathbf{k})\right|^2}{E_{j_2}(\mathbf{k})-E_{j_1}(\mathbf{k})}\\ &-\hat{\pi}_{j_1,j_1}(1;\mathbf{k})\hat{\pi}_{j_1,j_1}(2;\mathbf{k})\sum_{\substack{j_2=1\\ j_2\neq j_1}}^{\infty}\frac{2\Re\left(\hat{\pi}_{j_1,j_2}(2;\mathbf{k})\hat{\pi}_{j_2,j_1}(1;\mathbf{k})\right)}{E_{j_2}(\mathbf{k})-E_{j_1}(\mathbf{k})}\Bigg\}\end{aligned} \tag{3.21}$$

and

$$\mathfrak{a}_{j_1,2}(\mathbf{k}) := -\frac{1}{2!}\left\{ \sum_{\substack{j_2=1\\ j_2\neq j_1}}^{\infty} \sum_{\substack{j_3=1\\ j_3\neq j_1}}^{\infty} \frac{\mathcal{C}_{j_1,j_1,j_2,j_3}(\mathbf{k}) + \mathcal{C}_{j_1,j_2,j_1,j_3}(\mathbf{k}) + \mathcal{C}_{j_1,j_2,j_3,j_1}(\mathbf{k})}{(E_{j_2}(\mathbf{k}) - E_{j_1}(\mathbf{k}))\,(E_{j_3}(\mathbf{k}) - E_{j_1}(\mathbf{k}))} \right.$$
$$\left. + \sum_{\substack{j_2=1\\ j_2\neq j_1}}^{\infty} \frac{\mathcal{C}_{j_2,j_1,j_1,j_1}(\mathbf{k}) - \mathcal{C}_{j_1,j_1,j_2,j_1}(\mathbf{k})}{(E_{j_2}(\mathbf{k}) - E_{j_1}(\mathbf{k}))^2} \right\}. \tag{3.22}$$

Note that it is possible to identify in (3.20) all the functions $\mathfrak{a}_{j_1,l}(\cdot)$ for $j_1 \geq 1$ and $l \in \{1, 0\}$ since such a result is based only on identities provided by the residue theorem. However, the number of terms is large and we will not need their explicit expressions in order to prove our theorem.

Now we treat the next term.

Lemma 3.6. *The quantity defined by* (3.16) *can be rewritten as:*

$$\mathrm{Tr}_{L^2(\mathbb{R}^3)}\left\{\chi_\Omega \mathcal{W}_{\infty,2}(\beta,\mu_\infty)\right\}$$
$$= \frac{1}{4}\frac{1}{|\Omega^*|}\sum_{j_1=1}^{\infty}\int_{\Omega^*} \mathrm{d}\mathbf{k} \sum_{l=0}^{3} \frac{\partial^l \mathfrak{f}}{\partial \xi^l}\left(\beta,\mu_\infty; E_{j_1}(\mathbf{k})\right)\mathfrak{b}_{j_1,l}(\mathbf{k}) \tag{3.23}$$

where for all integers $j_1 \geq 1$ and all $\mathbf{k} \in \Omega^*$ we have:

$$\mathfrak{b}_{j_1,3}(\mathbf{k}) := \frac{1}{6}\left\{\left|\hat{\pi}_{j_1,j_1}(1;\mathbf{k})\right|^2 + \left|\hat{\pi}_{j_1,j_1}(2;\mathbf{k})\right|^2\right\}, \tag{3.24}$$

$$\mathfrak{b}_{j_1,2}(\mathbf{k}) := -\frac{1}{2}\sum_{\substack{j_2=1\\ j_2\neq j_1}}^{\infty} \frac{\left|\hat{\pi}_{j_1,j_2}(1;\mathbf{k})\right|^2 + \left|\hat{\pi}_{j_1,j_2}(2;\mathbf{k})\right|^2}{E_{j_2}(\mathbf{k}) - E_{j_1}(\mathbf{k})} + \frac{1}{2}, \tag{3.25}$$

$$\mathfrak{b}_{j_1,s}(\mathbf{k}) := -(2-s)\sum_{\substack{j_2=1\\ j_2\neq j_1}}^{\infty} \frac{\left|\hat{\pi}_{j_1,j_2}(1;\mathbf{k})\right|^2 + \left|\hat{\pi}_{j_1,j_2}(2;\mathbf{k})\right|^2}{(E_{j_2}(\mathbf{k}) - E_{j_1}(\mathbf{k}))^{3-s}}, \quad s \in \{0,1\}.$$

Thus our Lemmas 3.5 and 3.6 provide an expansion of the type announced in (3.1), where the coefficients are given by:

$$\mathfrak{c}_{j_1,l}(\mathbf{k}) := \mathfrak{a}_{j_1,l}(\mathbf{k}) + \mathfrak{b}_{j_1,l}(\mathbf{k}), \quad l \in \{0,1,2,3\}. \tag{3.26}$$

In particular, for all integer $j_1 \geq 1$ and for all $\mathbf{k} \in \Omega^*$, the functions $\mathfrak{c}_{j_1,3}(\cdot)$ and $\mathfrak{c}_{j_1,2}(\cdot)$ are respectively given by:

$$\mathfrak{c}_{j_1,3}(\mathbf{k}) := \frac{1}{3!}\Bigg\{ |\hat{\pi}_{j_1,j_1}(1;\mathbf{k})|^2 \Bigg(1 + \sum_{\substack{j_2=1 \\ j_2\neq j_1}}^{\infty} \frac{|\hat{\pi}_{j_1,j_2}(2;\mathbf{k})|^2}{E_{j_2}(\mathbf{k}) - E_{j_1}(\mathbf{k})}\Bigg)$$
$$+|\hat{\pi}_{j_1,j_1}(2;\mathbf{k})|^2 \Bigg(1 + \sum_{\substack{j_2=1 \\ j_2\neq j_1}}^{\infty} \frac{|\hat{\pi}_{j_1,j_2}(1;\mathbf{k})|^2}{E_{j_2}(\mathbf{k}) - E_{j_1}(\mathbf{k})}\Bigg)$$
$$-\hat{\pi}_{j_1,j_1}(1;\mathbf{k})\hat{\pi}_{j_1,j_1}(2;\mathbf{k}) \sum_{\substack{j_2=1 \\ j_2\neq j_1}}^{\infty} \frac{2\Re\left(\hat{\pi}_{j_1,j_2}(2;\mathbf{k})\hat{\pi}_{j_2,j_1}(1;\mathbf{k})\right)}{E_{j_2}(\mathbf{k}) - E_{j_1}(\mathbf{k})}\Bigg\} \tag{3.27}$$

and

$$\mathfrak{c}_{j_1,2}(\mathbf{k}) := -\frac{1}{2}\Bigg\{ \sum_{\substack{j_2=1 \\ j_2\neq j_1}}^{\infty} \frac{|\hat{\pi}_{j_1,j_2}(1;\mathbf{k})|^2 + |\hat{\pi}_{j_1,j_2}(2;\mathbf{k})|^2}{E_{j_2}(\mathbf{k}) - E_{j_1}(\mathbf{k})} - 1$$
$$+ \sum_{\substack{j_2=1 \\ j_2\neq j_1}}^{\infty} \frac{\mathcal{C}_{j_2,j_1,j_1,j_1}(\mathbf{k}) - \mathcal{C}_{j_1,j_1,j_2,j_1}(\mathbf{k})}{(E_{j_2}(\mathbf{k}) - E_{j_1}(\mathbf{k}))^2}$$
$$+ \sum_{\substack{j_2=1 \\ j_2\neq j_1}}^{\infty} \sum_{\substack{j_3=1 \\ j_3\neq j_1}}^{\infty} \frac{\mathcal{C}_{j_1,j_1,j_2,j_3}(\mathbf{k}) + \mathcal{C}_{j_1,j_2,j_1,j_3}(\mathbf{k}) + \mathcal{C}_{j_1,j_2,j_3,j_1}(\mathbf{k})}{(E_{j_2}(\mathbf{k}) - E_{j_1}(\mathbf{k}))(E_{j_3}(\mathbf{k}) - E_{j_1}(\mathbf{k}))}\Bigg\}, \tag{3.28}$$

where for all integers $j_1, j_2, j_3, j_4 \in \mathbb{N}^*, \Omega^* \ni \mathbf{k} \mapsto \mathcal{C}_{j_1,j_2,j_3,j_4}(\mathbf{k})$ is defined in (3.17).

In order to conclude the proof of Theorem 3.1, it remains to use this last result (its proof is in the appendix of this section):

Lemma 3.7. *For all integers $j_1 \geq 1$ and $l \in \{0, 1, 2, 3\}$, the maps $\Omega^* \ni \mathbf{k} \mapsto \mathfrak{a}_{j_1,l}(\mathbf{k})$ and $\Omega^* \ni \mathbf{k} \mapsto \mathfrak{b}_{j_1,l}(\mathbf{k})$ are bounded and continuous on any compact subset of Ω^* where E_{j_1} is isolated from the rest of the spectrum.*

Thus for all integers $j_1 \geq 1$ and $\mathbf{k} \in \Omega^*$, the maps $\mathfrak{c}_{j_1,l}(\cdot)$ appearing in (3.1) might be singular on a set with zero Lebesgue measure where E_{j_1} can touch the neighboring bands. However, the whole integrand in (3.1) is bounded and continuous on the whole Ω^* because it comes from two complex integrals ((3.15) and (3.16)) which do not have local singularities in $\mathbf{k}$.

3.4. Appendix—Proofs of the Intermediate Results

Here we prove Lemmas 3.5, 3.6, and 3.7.

Proof of Lemma 3.5. Let $\Omega^* \ni \mathbf{k} \mapsto \mathcal{C}_{j_1,j_2,j_3,j_4}(\mathbf{k})$ be the complex-valued function appearing in (3.15):

$$\begin{aligned}\mathcal{C}_{j_1,j_2,j_3,j_4}(\mathbf{k}) := & \{\hat{\pi}_{j_1,j_2}(1;\mathbf{k})\hat{\pi}_{j_2,j_3}(2;\mathbf{k}) - \hat{\pi}_{j_1,j_2}(2;\mathbf{k})\hat{\pi}_{j_2,j_3}(1;\mathbf{k})\} \\ & \times \{\hat{\pi}_{j_3,j_4}(2;\mathbf{k})\hat{\pi}_{j_4,j_1}(1;\mathbf{k}) - \hat{\pi}_{j_3,j_4}(1;\mathbf{k})\hat{\pi}_{j_4,j_1}(2;\mathbf{k})\}.\end{aligned} \tag{3.29}$$

Note that this function is identically zero for the following combinations of subscripts:

$$j_1 = j_2 = j_3 = j_4, \quad j_1 = j_2 = j_3 \neq j_4, \quad j_1 = j_3 = j_4 \neq j_2. \tag{3.30}$$

Therefore the expansion of (3.15) consists of partial derivatives of $\mathfrak{f}(\beta, \mu_\infty; \cdot\,)$ of order at most equal to three. On the other hand, since the functions $\mathcal{C}_{j_1,j_1,j_1,j_4}(\cdot\,)$ and $\mathcal{C}_{j_1,j_2,j_1,j_1}(\cdot\,)$ are identically equal to zero (see (3.30)), the quadruple summation in (3.15) is reduced to:

$$\begin{aligned}&\sum_{j_1,\ldots,j_4=1}^{\infty} \mathcal{C}_{j_1,j_2,j_3,j_4}(\mathbf{k}) \left(\frac{1}{2i\pi}\right) \\ &\quad \times \int_\Gamma \mathrm{d}\xi\, \frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{(E_{j_1}(\mathbf{k})-\xi)^2 (E_{j_2}(\mathbf{k})-\xi)(E_{j_3}(\mathbf{k})-\xi)(E_{j_4}(\mathbf{k})-\xi)} \\ &= \sum_{j_1=1}^{\infty} \sum_{\substack{j_3=1 \\ j_3\neq j_1}}^{\infty} \mathcal{C}_{j_1,j_1,j_3,j_1}(\mathbf{k}) \left(\frac{1}{2i\pi}\right) \int_\Gamma \mathrm{d}\xi\, \frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{(E_{j_1}(\mathbf{k})-\xi)^4 (E_{j_3}(\mathbf{k})-\xi)} \\ &\quad + \sum_{j_1=1}^{\infty} \sum_{\substack{j_2=1 \\ j_2\neq j_1}}^{\infty} \mathcal{C}_{j_1,j_2,j_2,j_2}(\mathbf{k}) \left(\frac{1}{2i\pi}\right) \int_\Gamma \mathrm{d}\xi\, \frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{(E_{j_1}(\mathbf{k})-\xi)^2 (E_{j_2}(\mathbf{k})-\xi)^3} \\ &\quad + \underbrace{\sum_{j_1,\ldots,j_4=1}^{\infty}}_{\substack{\text{at most 2 equal} \\ \text{subscripts}}} \mathcal{C}_{j_1,j_2,j_3,j_4}(\mathbf{k}) \left(\frac{1}{2i\pi}\right) \\ &\quad \times \int_\Gamma \mathrm{d}\xi\, \frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{(E_{j_1}(\mathbf{k})-\xi)^2 (E_{j_2}(\mathbf{k})-\xi)(E_{j_3}(\mathbf{k})-\xi)(E_{j_4}(\mathbf{k})-\xi)}.\end{aligned} \tag{3.31}$$

By applying the residue theorem in the first term of the right hand side of (3.31) we get:

$$\begin{aligned}&\sum_{\substack{j_3=1 \\ j_3\neq j_1}}^{\infty} \mathcal{C}_{j_1,j_1,j_3,j_1}(\mathbf{k}) \left(\frac{1}{2i\pi}\right) \int_\Gamma \mathrm{d}\xi\, \frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{(E_{j_1}(\mathbf{k})-\xi)^4 (E_{j_3}(\mathbf{k})-\xi)} \\ &\quad = \sum_{\substack{j_3=1 \\ j_3\neq j_1}}^{\infty} \mathcal{C}_{j_1,j_1,j_3,j_1}(\mathbf{k}) \left\{ \frac{1}{3!} \frac{1}{E_{j_3}(\mathbf{k}) - E_{j_1}(\mathbf{k})} \frac{\partial^3 \mathfrak{f}}{\partial \xi^3}(\beta,\mu_\infty; E_{j_1}(\mathbf{k}))\right.\end{aligned}$$

$$+\frac{3}{3!}\frac{1}{\left(E_{j_3}(\mathbf{k})-E_{j_1}(\mathbf{k})\right)^2}\frac{\partial^2\mathfrak{f}}{\partial\xi^2}\left(\beta,\mu_\infty;E_{j_1}(\mathbf{k})\right)$$
$$\left.+\text{others terms involving }\frac{\partial^l\mathfrak{f}}{\partial\xi^l}(\beta,\mu_\infty;\cdot),\text{ with } l\leq 1\right\}. \tag{3.32}$$

The function $\mathcal{C}_{j_1,j_1,j_3,j_1}(\cdot)$ appearing in front of $\frac{\partial^3\mathfrak{f}}{\partial\xi^3}\left(\beta,\mu_\infty;E_{j_1}(\mathbf{k})\right)$ in (3.32) corresponds to $\mathfrak{a}_{j_1,3}(\cdot)$ since:

$$\forall\,\mathbf{k}\in\Omega^*,\quad \mathcal{C}_{j_1,j_1,j_3,j_1}(\mathbf{k})=\left|\hat{\pi}_{j_1,j_1}(1;\mathbf{k})\hat{\pi}_{j_1,j_3}(2;\mathbf{k})-\hat{\pi}_{j_1,j_1}(2;\mathbf{k})\hat{\pi}_{j_1,j_3}(1;\mathbf{k})\right|^2.$$

Note that the function $\mathcal{C}_{j_1,j_1,j_3,j_1}(\cdot)$ contributes to the term $\mathfrak{a}_{j_1,2}(\cdot)$, too.

By applying once again the residue theorem in the second term of the right hand side of (3.31) we obtain:

$$\sum_{\substack{j_2=1\\ j_2\neq j_1}}^{\infty}\mathcal{C}_{j_1,j_2,j_2,j_2}(\mathbf{k})\left(\frac{1}{2i\pi}\right)\int_\Gamma \mathrm{d}\xi\,\frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{\left(E_{j_1}(\mathbf{k})-\xi\right)^2\left(E_{j_3}(\mathbf{k})-\xi\right)^3}$$
$$=\sum_{\substack{j_2=1\\ j_2\neq j_1}}^{\infty}\mathcal{C}_{j_1,j_2,j_2,j_2}(\mathbf{k})\left\{-\frac{1}{2!}\frac{1}{\left(E_{j_1}(\mathbf{k})-E_{j_2}(\mathbf{k})\right)^2}\frac{\partial^2\mathfrak{f}}{\partial\xi^2}\left(\beta,\mu_\infty;E_{j_2}(\mathbf{k})\right)\right.$$
$$\left.+\text{others terms involving }\frac{\partial^l\mathfrak{f}}{\partial\xi^l}(\beta,\mu_\infty;\cdot),\text{ with } l\leq 1\right\}. \tag{3.33}$$

The function $\mathcal{C}_{j_1,j_2,j_2,j_2}(\cdot)$ appearing in front of $\frac{\partial^2\mathfrak{f}}{\partial\xi^2}\left(\beta,\mu_\infty;E_{j_2}(\mathbf{k})\right)$ contributes to $\mathfrak{a}_{j_1,2}(\cdot)$.

It remains to isolate in (3.31) (where at most two subscripts are equal) all combinations which provide a second order derivative of $\mathfrak{f}(\beta,\mu_\infty;\cdot)$. These combinations are:

$$j_1=j_2\neq j_3,j_4;\quad j_1=j_3\neq j_2,j_4;\quad j_1=j_4\neq j_2,j_3.$$

Finally, we once again apply the residue theorem and gathering all terms proportional with $\frac{\partial^2\mathfrak{f}}{\partial\xi^2}(\beta,\mu_\infty;\cdot)$. The proof is over. □

Proof of Lemma 3.6. By separating the cases $j_1=j_2$ and $j_1\neq j_2$, the double summation in the right hand side of (3.16) reads as:

$$\sum_{j_1=1}^{\infty}\sum_{j_2=1}^{\infty}\mathcal{C}_{j_1,j_2}(\mathbf{k})\left(\frac{1}{2i\pi}\right)\int_\Gamma \mathrm{d}\xi\,\frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{\left(E_{j_1}(\mathbf{k})-\xi\right)^3\left(E_{j_2}(\mathbf{k})-\xi\right)}$$
$$=\sum_{j_1=1}^{\infty}\mathcal{C}_{j_1,j_1}(\mathbf{k})\left(\frac{1}{2i\pi}\right)\int_\Gamma \mathrm{d}\xi\,\frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{\left(E_{j_1}(\mathbf{k})-\xi\right)^4}$$
$$+\sum_{j_1=1}^{\infty}\sum_{\substack{j_2=1\\ j_2\neq j_1}}^{\infty}\mathcal{C}_{j_1,j_2}(\mathbf{k})\left(\frac{1}{2i\pi}\right)\int_\Gamma \mathrm{d}\xi\,\frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{\left(E_{j_1}(k)(\mathbf{k})-\xi\right)^3\left(E_{j_2}(\mathbf{k})-\xi\right)}. \tag{3.34}$$

By using the residue theorem in the first term of the r.h.s. of (3.34):

$$\left(\frac{1}{2i\pi}\right)\int_\Gamma \mathrm{d}\xi\, \frac{\mathfrak{f}(\beta,\mu_\infty;\xi)}{(E_{j_1}(\mathbf{k})-\xi)^4} = \frac{1}{3!}\frac{\partial^3 \mathfrak{f}}{\partial\xi^3}\,(\beta,\mu_\infty;E_{j_1}(\mathbf{k}))$$

This is only the one term which provides a third-order partial derivative of $\mathfrak{f}(\beta,\mu_\infty;\cdot)$. The rest of the proof is just plain computation using the residue theorem. We do not give further details. □

Proof of Lemma 3.7. Let $p_\alpha := -i\partial_\alpha$ be the α component of the momentum operator with periodic boundary conditions in $L^2(\Omega), \alpha\in\{1,2,3\}$. Now assume that $E_{j_1}(\mathbf{k})$ is isolated and non-degenerate if $\mathbf{k}$ belongs to some compact $K\subset\Omega^*$. We have to investigate integrals of the type

$$\mathrm{Tr}_{L^2(\Omega)}\int_\Gamma \mathrm{d}\xi\,\mathfrak{f}(\beta,\mu_\infty;\xi)(h(\mathbf{k})-\xi)^{-1}p_{\alpha_1}(h(\mathbf{k})-\xi)^{-1}\cdots p_{\alpha_4}(h(\mathbf{k})-\xi)^{-1}. \tag{3.35}$$

Let $\mathbf{k}_0\in K$, and let Γ_1 be a simple, positively oriented path surrounding $E_{j_1}(\mathbf{k}_0)$ but no other eigenvalue of $h(\mathbf{k}_0)$. If $|\mathbf{k}-\mathbf{k}_0|$ is small enough, Γ_1 will still only contain $E_{j_1}(\mathbf{k})$. The projection $\Pi(\mathbf{k})$ corresponding to $E_{j_1}(\mathbf{k})$ is given by a Riesz integral. We have:

$$\Pi(\mathbf{k}) = \frac{i}{2\pi}\int_{\Gamma_1}\mathrm{d}z\,(h(\mathbf{k})-z)^{-1}, \tag{3.36}$$

and is continuous at $\mathbf{k}_0$ in the trace norm topology. Moreover,

$$\begin{aligned}\Pi(\mathbf{k})(h(\mathbf{k})-\xi)^{-1} &= \frac{1}{E_{j_1}(\mathbf{k})-\xi}\Pi(\mathbf{k}),\\ (\mathbf{1}-\Pi(\mathbf{k}))(h(\mathbf{k})-\xi)^{-1} &= \frac{1}{2\pi i}\int_{\Gamma_1}\mathrm{d}z\,\frac{1}{z-\xi}(h(\mathbf{k})-z)^{-1}.\end{aligned} \tag{3.37}$$

Clearly, $\Pi(\mathbf{k})(h(\mathbf{k})-\xi)^{-1}$ is analytic in ξ in the exterior of Γ_1. We can decompose the integral on Γ in (3.35) as a sum of three integrals, one of which being on a simple contour Γ_2 around $E_{j_1}(\mathbf{k}_0)$, completely surrounded by Γ_1. The other two integrals will never have $E_{j_1}(\mathbf{k})$ as a singularity, so they cannot contribute to the formula of $\mathfrak{a}_{j_1,l}(\mathbf{k})$. On the other hand, in the integral on Γ_2 we can replace the resolvents with the decomposition in (3.37) and use the fact that $(\mathbf{1}-\Pi(\mathbf{k}))(h(\mathbf{k})-\xi)^{-1}$ is analytic if ξ lies inside Γ_2. Now one can apply the Cauchy residue formula. For example, we can compute the integral in which we have $\Pi(\mathbf{k})$ at the extremities, and $(\mathbf{1}-\Pi(\mathbf{k}))$ in the interior; in that case $E_{j_1}=E_{j_1}(\mathbf{k})$ will be a double pole:

$$\begin{aligned}&\mathrm{Tr}_{L^2(\Omega)}\int_{\Gamma_2}\mathrm{d}\xi\,\mathfrak{f}(\xi)\Pi(\mathbf{k})(h(\mathbf{k})-\xi)^{-1}p_{\alpha_1}(h(\mathbf{k})-\xi)^{-1}\\ &\quad\times(\mathbf{1}-\Pi(\mathbf{k}))\cdots p_{\alpha_4}(h(\mathbf{k})-\xi)^{-1}\Pi(\mathbf{k}) = 2\pi i\Big\{(\partial_\xi\mathfrak{f})(E_{j_1}(\mathbf{k}))\mathrm{Tr}_{L^2(\Omega)}\\ &\quad\times\big\{\Pi(\mathbf{k})p_{\alpha_1}(h(\mathbf{k})-E_{j_1})^{-1}(\mathbf{1}-\Pi(\mathbf{k}))\cdots p_{\alpha_4}\Pi(\mathbf{k})\big\}\end{aligned}$$

$$+\mathfrak{f}(E_{j_1}(\mathbf{k}))\frac{d}{d\xi}\mathrm{Tr}_{L^2(\Omega)}\left\{\Pi(\mathbf{k})p_{\alpha_1}(h(\mathbf{k})-\xi)^{-1}(\mathbf{1}-\Pi(\mathbf{k}))\cdots(h(\mathbf{k})-\xi)^{-1}\right.$$
$$\left.\times(\mathbf{1}-\Pi(\mathbf{k}))p_{\alpha_4}\right\}_{\xi=E_{j_1}(\mathbf{k})}\Bigg\}. \tag{3.38}$$

Thus one contribution to $\mathfrak{a}_{j_1,1}(\mathbf{k})$ will be:

$$\mathrm{Tr}_{L^2(\Omega)}\left\{\Pi(\mathbf{k})p_{\alpha_1}(h(\mathbf{k})-E_{j_1})^{-1}(\mathbf{1}-\Pi(\mathbf{k}))\cdots p_{\alpha_4}\Pi(\mathbf{k})\right\}.$$

This expression does not use eigenvectors, only resolvents and projectors. Since E_{j_1} is continuous at $\mathbf{k}_0$, the map

$$\mathbf{k}\mapsto(\mathbf{1}-\Pi(\mathbf{k}))(h(\mathbf{k})-E_{j_1}(\mathbf{k}))^{-1}=\frac{1}{2\pi i}\int_{\Gamma_1}\mathrm{d}z\,\frac{1}{z-E_{j_1}(\mathbf{k})}(h(\mathbf{k})-z)^{-1}$$

is operator norm continuous at $\mathbf{k}_0$, and the map $\mathbf{k}\mapsto\Pi(\mathbf{k})$ is continuous in the trace norm. By using standard perturbation theory (see e.g. [25]), the same holds for the maps:

$$\mathbf{k}\mapsto(\mathbf{1}-\Pi(\mathbf{k}))(h(\mathbf{k})-E_{j_1}(\mathbf{k}))^{-1}p_{\alpha_l}$$

and

$$\mathbf{k}\mapsto p_{\alpha_l}(\mathbf{1}-\Pi(\mathbf{k}))(h(\mathbf{k})-E_{j_1}(\mathbf{k}))^{-1}p_{\alpha_k}.$$

Thus the trace defines a continuous function; all other coefficients can be treated in a similar way. □

4. The Zero-Field Susceptibility at Fixed Density and Zero Temperature

In this section, we separately investigate the semiconducting and metallic cases from the expansion (3.1). In particular, we prove Theorem 1.2 (i) and (ii).

4.1. The Semiconducting Case (SC)—Proof of Theorem 1.2 (i)

By using that $\mathfrak{f}_{FD}(\beta,\mu;\xi)=-\beta^{-1}\partial_\xi\mathfrak{f}(\beta,\mu;\xi)$, (3.1) can be rewritten as:

$$\mathcal{X}(\beta,\rho_0)=\left(\frac{\mathrm{e}}{c}\right)^2\frac{1}{2}\frac{1}{(2\pi)^3}\sum_{j_1=1}^{\infty}\int_{\Omega^*}\mathrm{d}\mathbf{k}\left\{\sum_{l=0}^{2}\frac{\partial^l\mathfrak{f}_{FD}}{\partial\xi^l}(\beta,\mu_\infty;E_{j_1}(\mathbf{k}))\,\mathfrak{c}_{j_1,1+l}(\mathbf{k})\right.$$
$$\left.-\frac{1}{\beta}\mathfrak{f}(\beta,\mu_\infty;E_{j_1}(\mathbf{k}))\,\mathfrak{c}_{j_1,0}(\mathbf{k})\right\}. \tag{4.1}$$

From (4.1), the proof of Theorem 1.2 (i) is based on two main ingredients. The first one is that for any fixed $\mu\geq E_0$ we have the following pointwise convergences:

$$\begin{aligned}&\lim_{\beta\to\infty}\frac{1}{\beta}\mathfrak{f}(\beta,\mu;\xi)=(\mu-\xi)\chi_{[E_0,\mu]}(\xi),\\&\lim_{\beta\to\infty}\mathfrak{f}_{FD}(\beta,\mu;\xi)=\chi_{[E_0,\mu]}(\xi),\quad\forall\,\xi\in[E_0,\infty)\setminus\{\mu\},\end{aligned} \tag{4.2}$$

while in the distributional sense:

$$\lim_{\beta\to\infty}\frac{\partial\mathfrak{f}_{FD}}{\partial\xi}(\beta,\mu;\xi)=-\delta(\xi-\mu),\quad \lim_{\beta\to\infty}\frac{\partial^2\mathfrak{f}_{FD}}{\partial\xi^2}(\beta,\mu;\xi)=-\partial_\xi\delta(\xi-\mu). \tag{4.3}$$

The second ingredient is related to the decay of the derivatives of the Fermi-Dirac distribution: for all $d>0$ and for all $j\in\mathbb{N}^*$, there exists a constant $C_{j,d}>0$ such that

$$\sup_{|\xi-\mu|\geq d>0}\left|\frac{\partial^j\mathfrak{f}_{FD}}{\partial\xi^j}(\beta,\mu;\xi)\right|\leq C_{j,d}\mathrm{e}^{-\frac{\beta|\xi-\mu|}{2}}. \tag{4.4}$$

Now assume that we are in the semiconducting case with a non-trivial gap, that is there exists $N\in\mathbb{N}^*$ such that $\lim_{\beta\to\infty}\mu_\infty(\beta,\rho_0)=(\max\mathcal{E}_N+\min\mathcal{E}_{N+1})/2=\mathcal{E}_F(\rho_0)$ and $\max\mathcal{E}_N<\min\mathcal{E}_{N+1}$. Since the Fermi energy lies inside a gap, all terms containing derivatives of the Fermi–Dirac distribution will converge to zero in the limit $\beta\to\infty$. Here (4.4) plays a double important role: first, it makes the series in j_1 convergent, and second, it provides an exponential decay to zero. Then by taking into account (4.2), we immediately get (1.15) from (4.1). □

4.2. The Metallic Case (M)—Proof of Theorem 1.2 (ii)

Now we are interested in the metallic case. The limit $\beta\to\infty$ is not so simple as in the previous case, because the Fermi energy lies in the spectrum. The starting point is the same formula (3.1), but we have to modify it by getting rid of the third order partial derivatives of $\mathfrak{f}$ in order to make appear a Landau-Peierls type contribution. However, this operation needs the already announced additional assumption of non-degeneracy (which will provide regularity in $\mathbf{k}$) in a neighborhood of the Fermi surface:

Assumption 4.1. *We assume that there exists a unique $N\in\mathbb{N}^*$ such that $\lim_{\beta\to\infty}\mu_\infty(\beta,\rho_0)=\mathcal{E}_F(\rho_0)\in(\min\mathcal{E}_N,\max\mathcal{E}_N)$, which means that the Fermi energy lies inside the Nth Bloch band $\mathcal{E}_N$. We also assume that the Fermi surface defined by $\mathcal{S}_F:=\{\mathbf{k}\in\Omega^*:E_N(\mathbf{k})=\mathcal{E}_F(\rho_0)\}$ is smooth and non-degenerate.*

Recall that $E_N(\mathbf{k})$ is supposed to be non degenerate outside a (possibly empty) zero Lebesgue measure set of $\mathbf{k}$-points. Our assumption leads to the following consequence:

$$\operatorname{dist}\left\{\mathcal{E}_F(\rho_0),\cup_{j=1}^{N-1}\mathcal{E}_j\right\}=d_1>0,\quad \operatorname{dist}\left\{\mathcal{E}_F(\rho_0),\cup_{j=N+1}^{\infty}\mathcal{E}_j\right\}=d_2>0. \tag{4.5}$$

Note that the minimum of the lowest Bloch band $\mathcal{E}_1$ is always simple. If the density ρ_0 is small enough then Assumption 4.1 is automatically satisfied since the Bloch energy function $\mathbf{k}\mapsto E_1(\mathbf{k})$ is non-degenerate in a neighborhood of $\mathbf{k}=\mathbf{0}$ (see e.g. [28]).

In fact, the non-degeneracy assumption is indispensable for to use of the regular perturbation theory in order to express the functions defined by (3.24), (3.25) and (3.21) (only in the case where $j_1=N$) with the help of the partial derivatives of $E_N(\cdot)$ with respect to the k_i-variables, for $\mathbf{k}$ in a neighborhood of the Fermi surface:

$$\frac{\partial E_N(\mathbf{k})}{\partial k_i} = \hat{\pi}_{N,N}(i;\mathbf{k}), \quad i \in \{1,2,3\}, \tag{4.6}$$

$$\frac{\partial^2 E_N(\mathbf{k})}{\partial k_i^2} = 1 + 2\sum_{\substack{j=1\\ j\neq N}}^{\infty} \frac{\left|\hat{\pi}_{j,N}(i;\mathbf{k})\right|^2}{E_N(\mathbf{k}) - E_j(\mathbf{k})}, \quad i \in \{1,2,3\}, \tag{4.7}$$

$$\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2} = \sum_{\substack{j=1\\ j\neq N}}^{\infty} \frac{2\Re\left\{\hat{\pi}_{j,N}(1;\mathbf{k})\hat{\pi}_{N,j}(2;\mathbf{k})\right\}}{E_N(\mathbf{k}) - E_j(\mathbf{k})} = \frac{\partial^2 E_N(\mathbf{k})}{\partial k_2 \partial k_1}. \tag{4.8}$$

Such identities have been studied in [16]. Note that the above series are absolutely convergent if the potential V is smooth enough ([16]).

Now using Assumption 4.1, we can group the coefficients corresponding to the third and second order derivatives of $\mathfrak{f}$ appearing in (3.1). This operation allows us to isolate a Landau-Peierls type contribution (the proof can be found in the appendix of this section):

Proposition 4.2. *Assume for simplicity that $\mathcal{E}_N$ is a simple band. Let $\Omega^* \ni \mathbf{k} \mapsto \mathfrak{c}_{N,2}(\mathbf{k})$ and $\Omega^* \ni \mathbf{k} \mapsto \mathfrak{c}_{N,3}(\mathbf{k})$ the functions respectively defined by (3.28) and (3.27) with $j_1 = N$. Then:*

$$\int_{\Omega^*} d\mathbf{k} \sum_{l=2}^{3} \frac{\partial^l \mathfrak{f}}{\partial \xi^l}(\beta,\mu_\infty;E_N(\mathbf{k}))\,\mathfrak{c}_{N,l}(\mathbf{k}) = \int_{\Omega^*} d\mathbf{k}\, \frac{\partial^2 \mathfrak{f}}{\partial \xi^2}(\beta,\mu_\infty;E_N(\mathbf{k})) \times \left\{\frac{1}{3!}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2}\,\frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} - \frac{1}{3!}\left(\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2}\right)^2 + \mathfrak{a}_{N,2}(\mathbf{k})\right\}, \tag{4.9}$$

where $\Omega^* \ni \mathbf{k} \mapsto \mathfrak{a}_{j_1,2}(\mathbf{k})$ are the functions defined in (3.22).

From (3.1) and Proposition 4.2 we get an expansion for the orbital susceptibility at fixed density $\rho_0 > 0$ and inverse of temperature $\beta > 0$:

Proposition 4.3. *Assume for simplicity that $\mathcal{E}_N$ is a simple band. For every $j_1 \in \mathbb{N}^*$ there exist four families of functions $\mathfrak{c}_{j_1,l}(\cdot)$ with $l \in \{0,1,2,3\}$, defined on Ω^* outside a set of Lebesgue measure zero, such that the second integrand below is bounded and continuous on Ω^*:*

$$\mathcal{X}(\beta,\rho_0) = -\left(\frac{e}{c}\right)^2 \frac{1}{12\beta}\frac{1}{(2\pi)^3} \cdot\left\{\int_{\Omega^*} d\mathbf{k}\, \frac{\partial^2 \mathfrak{f}}{\partial \xi^2}(\beta,\mu_\infty;E_N(\mathbf{k}))\left[\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} - \left(\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2}\right)^2 - 3\mathcal{F}_N(\mathbf{k})\right]\right.$$

$$+6 \int_{\Omega^*} \mathrm{d}\mathbf{k} \left[\sum_{\substack{j_1=1 \\ j_1 \neq N}}^{\infty} \sum_{l=2}^{3} \frac{\partial^l \mathfrak{f}}{\partial \xi^l} \left(\beta, \mu_\infty; E_{j_1}(\mathbf{k})\right) \mathfrak{c}_{j_1,l}(\mathbf{k}) \right.$$

$$\left. + \sum_{j_1=1}^{\infty} \sum_{l=0}^{1} \frac{\partial^l \mathfrak{f}}{\partial \xi^l} \left(\beta, \mu_\infty; E_{j_1}(\mathbf{k})\right) \mathfrak{c}_{j_1,l}(\mathbf{k}) \right] \Bigg\}, \tag{4.10}$$

where by convention $(\partial_\xi^0 \mathfrak{f})(\beta, \mu_\infty; \cdot) := \mathfrak{f}(\beta, \mu_\infty; \cdot)$ *and*:

$$\begin{aligned} \mathcal{F}_N(\mathbf{k}) &:= -2\mathfrak{a}_{N,2}(\mathbf{k}) \\ &= \sum_{\substack{j_2=1 \\ j_2 \neq N}}^{\infty} \sum_{\substack{j_3=1 \\ j_3 \neq N}}^{\infty} \frac{\mathcal{C}_{N,N,j_2,j_3}(\mathbf{k}) + \mathcal{C}_{N,j_2,N,j_3}(\mathbf{k}) + \mathcal{C}_{N,j_2,j_3,N}(\mathbf{k})}{\left(E_{j_2}(\mathbf{k}) - E_N(\mathbf{k})\right)\left(E_{j_3}(\mathbf{k}) - E_N(\mathbf{k})\right)} \\ &\quad + \sum_{\substack{j_2=1 \\ j_2 \neq N}}^{\infty} \frac{\mathcal{C}_{j_2,N,N,N}(\mathbf{k}) - \mathcal{C}_{N,N,j_2,N}(\mathbf{k})}{\left(E_{j_2}(\mathbf{k}) - E_N(\mathbf{k})\right)^2}. \end{aligned} \tag{4.11}$$

Note that we can use identities provided by the regular perturbation theory in order to express the functions $\mathfrak{c}_{j_1,l}$ (as well as $\mathcal{F}_N$) appearing in (4.10) in terms of derivatives of E_j and u_j w.r.t. the $\mathbf{k}$-variable. But this formulation will only hold true outside a set of $\mathbf{k}$-points of Lebesgue measure zero, while the formulation involving $\hat{\pi}_{i,j}$'s is more general, physically relevant, providing us with bounded and continuous coefficients on Ω^* (see Lemma 3.7). Finally keep in mind that the main goal is the Landau-Peierls formula, and it will turn out that only the factor multiplying the second partial derivative of $\mathfrak{f}$ will contribute to it.

In order to complete the proof of Theorem 1.2 (*ii*), it remains to take the limit when $\beta \to \infty$ in (4.10). Since the Fermi energy lies inside the band $\mathcal{E}_N$ and it is isolated from all other bands, then using (4.3) and (4.4) we have:

$$\lim_{\beta \to \infty} \frac{1}{\beta} \int_{\Omega^*} \mathrm{d}\mathbf{k} \sum_{\substack{j=1 \\ j \neq N}}^{\infty} \sum_{l=2}^{3} \frac{\partial^l \mathfrak{f}}{\partial \xi^l}(\beta, \mu_\infty(\beta, \rho_0); E_j(\mathbf{k}))\mathfrak{c}_{j,l}(\mathbf{k}) = 0$$

and

$$\begin{aligned} &\lim_{\beta \to \infty} -\frac{1}{\beta} \int_{\Omega^*} \mathrm{d}\mathbf{k} \, \frac{\partial^2 \mathfrak{f}}{\partial \xi^2}(\beta, \mu_\infty; E_N(\mathbf{k})) \\ &\qquad \times \left\{ \frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2} \frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} - \left(\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2} \right)^2 - 3\mathcal{F}_N(\mathbf{k}) \right\} \\ &= -\int_{\mathcal{S}_F} \frac{\mathrm{d}\sigma(\mathbf{k})}{|\nabla E_N(\mathbf{k})|} \left\{ \frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2} \frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} - \left(\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2} \right)^2 - 3\mathcal{F}_N(\mathbf{k}) \right\} \end{aligned}$$

where $\mathcal{S}_F$ denotes the Fermi surface. Using these two identities together with (4.2) in (4.10), we obtain (1.16).

4.3. Appendix—Proof of Proposition 4.2

Using (3.26) we get:

$$\int_{\Omega^*} \mathrm{d}\mathbf{k} \sum_{l=2}^{3} \frac{\partial^l \mathfrak{f}}{\partial \xi^l} (\beta, \mu_\infty; E_N(\mathbf{k}))\, \mathfrak{c}_{N,l}(\mathbf{k}) = \int_{\Omega^*} \mathrm{d}\mathbf{k} \frac{\partial^2 \mathfrak{f}}{\partial \xi^2} (\beta, \mu_\infty; E_N(\mathbf{k}))\, \mathfrak{a}_{N,2}(\mathbf{k})$$
$$+ \int_{\Omega^*} \mathrm{d}\mathbf{k} \left[\sum_{l=2}^{3} \frac{\partial^l \mathfrak{f}}{\partial \xi^l} (\beta, \mu_\infty; E_N(\mathbf{k}))\, \mathfrak{b}_{N,l}(\mathbf{k}) + \frac{\partial^3 \mathfrak{f}}{\partial \xi^3} (\beta, \mu_\infty; E_N(\mathbf{k}))\, \mathfrak{a}_{N,3}(\mathbf{k}) \right].$$

Using (4.6) and (4.7), the functions $\mathfrak{b}_{N,l}(\cdot), l \in \{2,3\}$, can be rewritten as:

$$\mathfrak{b}_{N,3}(\mathbf{k}) = \frac{1}{3!} \left\{ \left(\frac{\partial E_N(\mathbf{k})}{\partial k_1} \right)^2 + \left(\frac{\partial E_N(\mathbf{k})}{\partial k_2} \right)^2 \right\},$$
$$\mathfrak{b}_{N,2}(\mathbf{k}) = -\frac{1}{2!} \left\{ -\frac{1}{2} \left(\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2} - 1 \right) - \frac{1}{2} \left(\frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} - 1 \right) - 1 \right\}$$
$$= \frac{1}{2!} \frac{1}{2} \left\{ \frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2} + \frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} \right\}.$$

Since $E_N(\cdot) \in \mathcal{C}^2(\mathbb{R}^3/(2\pi\mathbb{Z}^3))$, a simple integration by parts gives us:

$$\forall\, i \in \{1,2\}, \quad \int_{-\pi}^{\pi} \mathrm{d}k_i \frac{\partial E_N(\mathbf{k})}{\partial k_i} \frac{\partial \mathfrak{f}^3}{\partial \xi^3} (\beta, \mu_\infty; E_N(\mathbf{k})) \frac{\partial E_N(\mathbf{k})}{\partial k_i}$$
$$= - \int_{-\pi}^{\pi} \mathrm{d}k_i \frac{\partial \mathfrak{f}^2}{\partial \xi^2} (\beta, \mu_\infty; E_N(\mathbf{k})) \frac{\partial^2 E_N(\mathbf{k})}{\partial k_i^2} \tag{4.12}$$

whence:

$$\int_{\Omega^*} \mathrm{d}\mathbf{k} \frac{\partial^3 \mathfrak{f}}{\partial \xi^3} (\beta, \mu_\infty; E_N(\mathbf{k}))\, \mathfrak{b}_{N,3}(\mathbf{k})$$
$$= -\frac{1}{3!} \int_{\Omega^*} \mathrm{d}\mathbf{k} \frac{\partial^2 \mathfrak{f}}{\partial \xi^2} (\beta, \mu_\infty; E_N(\mathbf{k})) \left\{ \frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2} + \frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} \right\}$$

and:

$$\int_{\Omega^*} \mathrm{d}\mathbf{k} \sum_{l=2}^{3} \frac{\partial^l \mathfrak{f}}{\partial \xi^l} (\beta, \mu_\infty; E_N(\mathbf{k}))\, \mathfrak{b}_{N,l}(\mathbf{k})$$
$$= \frac{1}{3!} \frac{1}{2} \int_{\Omega^*} \mathrm{d}\mathbf{k} \frac{\partial^2 \mathfrak{f}}{\partial \xi^2} (\beta, \mu_\infty; E_N(\mathbf{k})) \left\{ \frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2} + \frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} \right\} \tag{4.13}$$

On the other hand, using (4.6), (4.7) and (4.8), the function $\mathfrak{a}_{N,3}(\cdot\,)$ can be rewritten as:

$$\begin{aligned}
&\mathfrak{a}_{N,3}(\mathbf{k})\\
&\quad= \frac{1}{3!}\left\{\left(\frac{\partial E_N(\mathbf{k})}{\partial k_1}\right)^2 \frac{1}{2}\left(1-\frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2}\right)+\left(\frac{\partial E_N(\mathbf{k})}{\partial k_2}\right)^2 \frac{1}{2}\left(1-\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2}\right)\right.\\
&\qquad\left.-\left(\frac{\partial E_N(\mathbf{k})}{\partial k_1}\right)\left(\frac{\partial E_N(\mathbf{k})}{\partial k_2}\right)\left(-\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2}\right)\right\}. \qquad (4.14)
\end{aligned}$$

Note that by a simple integration by parts:

$$\begin{aligned}
&\forall\, i \neq j \in \{1,2\}, \quad \int_{-\pi}^{\pi} \mathrm{d}k_j\, \frac{\partial E_N(\mathbf{k})}{\partial k_j}\frac{\partial^3 \mathfrak{f}}{\partial \xi^3}(\beta,\mu_\infty;E_N(\mathbf{k}))\,\frac{\partial E_N(\mathbf{k})}{\partial k_j}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_i^2}\\
&\quad= -\int_{-\pi}^{\pi} \mathrm{d}k_j\, \frac{\partial^2 \mathfrak{f}}{\partial \xi^2}(\beta,\mu_\infty;E_N(\mathbf{k}))\,\frac{\partial}{\partial k_j}\left[\frac{\partial E_N(\mathbf{k})}{\partial k_j}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_i^2}\right]\\
&\quad= -\int_{-\pi}^{\pi} \mathrm{d}k_j\, \frac{\partial^2 \mathfrak{f}}{\partial \xi^2}(\beta,\mu_\infty;E_N(\mathbf{k}))\\
&\qquad\times\left\{\frac{\partial^2 E_N(\mathbf{k})}{\partial k_j^2}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_i^2}+\frac{\partial E_N(\mathbf{k})}{\partial k_j}\frac{\partial}{\partial k_j}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_i^2}\right\}\\
&\quad= -\int_{-\pi}^{\pi} \mathrm{d}k_j\, \frac{\partial^2 \mathfrak{f}}{\partial \xi^2}(\beta,\mu_\infty;E_N(\mathbf{k}))\\
&\qquad\times\left\{\frac{\partial^2 E_N(\mathbf{k})}{\partial k_j^2}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_i^2}+\frac{\partial E_N(\mathbf{k})}{\partial k_j}\frac{\partial}{\partial k_i}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_j \partial k_i}\right\}. \qquad (4.15)
\end{aligned}$$

By virtue of (4.14), using (4.15) and (4.12), we get:

$$\begin{aligned}
&\int_{\Omega^*} \mathrm{d}\mathbf{k}\, \frac{\partial^3 \mathfrak{f}}{\partial \xi^3}(\beta,\mu_\infty;E_N(\mathbf{k}))\,\mathfrak{a}_{N,3}(\mathbf{k}) = \frac{1}{3!}\frac{1}{2}\int_{\Omega^*} \mathrm{d}\mathbf{k}\, \frac{\partial^2 \mathfrak{f}}{\partial \xi^2}(\beta,\mu_\infty;E_N(\mathbf{k}))\\
&\qquad\times\left\{2\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2}+\frac{\partial E_N(\mathbf{k})}{\partial k_1}\frac{\partial}{\partial k_2}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2}\right.\\
&\qquad\left.+\frac{\partial E_N(\mathbf{k})}{\partial k_2}\frac{\partial}{\partial k_1}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_2 \partial k_1}-\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2}-\frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2}\right\}\\
&\qquad+\frac{1}{3!}\int_{\Omega^*} \mathrm{d}\mathbf{k}\, \frac{\partial^3 \mathfrak{f}}{\partial \xi^3}(\beta,\mu_\infty;E_N(\mathbf{k}))\,\frac{\partial E_N(\mathbf{k})}{\partial k_1}\frac{\partial E_N(\mathbf{k})}{\partial k_2}\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2}. \qquad (4.16)
\end{aligned}$$

Finally, by a last integration by parts:

$$\forall i \neq j \in \{1,2\}, \quad \int_{-\pi}^{\pi} \mathrm{d}k_j \, \frac{\partial E_N(\mathbf{k})}{\partial k_j} \frac{\partial^2 \mathfrak{f}}{\partial \xi^2} (\beta, \mu_\infty; E_N(\mathbf{k})) \, \frac{\partial}{\partial k_i} \frac{\partial^2 E_N(\mathbf{k})}{\partial k_j \partial k_i}$$

$$= - \int_{-\pi}^{\pi} \mathrm{d}k_j \, \frac{\partial}{\partial k_i} \left[\frac{\partial E_N(\mathbf{k})}{\partial k_j} \frac{\partial^2 \mathfrak{f}}{\partial \xi^2} (\beta, \mu_\infty; E_N(\mathbf{k})) \right] \frac{\partial^2 E_N(\mathbf{k})}{\partial k_j \partial k_i}$$

$$= - \int_{-\pi}^{\pi} \mathrm{d}k_j \, \left\{ \frac{\partial^2 E_N(\mathbf{k})}{\partial k_i \partial k_j} \frac{\partial^2 \mathfrak{f}}{\partial \xi^2} (\beta, \mu_\infty; E_N(\mathbf{k})) \right.$$

$$\left. + \frac{\partial E_N(\mathbf{k})}{\partial k_j} \frac{\partial E_N(\mathbf{k})}{\partial k_i} \frac{\partial^3 \mathfrak{f}}{\partial \xi^3} (\beta, \mu_\infty; E_N(\mathbf{k})) \right\} \frac{\partial^2 E_N(\mathbf{k})}{\partial k_j \partial k_i}.$$

Then (4.16) is reduced to:

$$\int_{\Omega^*} \mathrm{d}\mathbf{k} \, \frac{\partial^3 \mathfrak{f}}{\partial \xi^3} (\beta, \mu_\infty; E_N(\mathbf{k})) \, \mathfrak{a}_{N,3}(\mathbf{k}) = \frac{1}{3!} \frac{1}{2} \int_{\Omega^*} \mathrm{d}\mathbf{k} \, \frac{\partial^2 \mathfrak{f}}{\partial \xi^2} (\beta, \mu_\infty; E_N(\mathbf{k}))$$
$$\times \left\{ 2 \frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2} \frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} - 2 \left(\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2} \right)^2 - \frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2} - \frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} \right\}. \tag{4.17}$$

By adding (4.13) to (4.17) we get:

$$\int_{\Omega^*} \mathrm{d}\mathbf{k} \left[\sum_{l=2}^{3} \frac{\partial^l \mathfrak{f}}{\partial \xi^l} (\beta, \mu_\infty; E_N(\mathbf{k})) \, \mathfrak{b}_{N,l}(\mathbf{k}) + \frac{\partial^3 \mathfrak{f}}{\partial \xi^3} (\beta, \mu_\infty; E_N(\mathbf{k})) \, \mathfrak{a}_{N,3}(\mathbf{k}) \right]$$
$$= \frac{1}{3!} \int_{\Omega^*} \mathrm{d}\mathbf{k} \, \frac{\partial^2 \mathfrak{f}}{\partial \xi^2} (\beta, \mu_\infty; E_N(\mathbf{k})) \left\{ \frac{\partial^2 E_N(\mathbf{k})}{\partial k_1^2} \frac{\partial^2 E_N(\mathbf{k})}{\partial k_2^2} - \left(\frac{\partial^2 E_N(\mathbf{k})}{\partial k_1 \partial k_2} \right)^2 \right\}$$

and we are done. Note that the proof does not work if E_N can touch other bands because we loose regularity. In that case the integration by parts have to be done across a tubular neighborhood of the Fermi surface $\mathcal{S}_F$, the price being the apparition of some extra terms. These terms will though disappear in the limit $\beta \to \infty$ because they will decay exponentially with β. □

5. The Landau-Peierls Formula

The aim of this section is to establish an asymptotic expansion of (1.16) in the limit of small densities ($\rho_0 \to 0$). Here we prove the expansion (1.17), of which (1.18) is a particular case which has already been suggested by Kjeldaas and Kohn in 1957 [26].

5.1. Proof of Theorem 1.2 (iii)

Let us recall that $E_0 = \min_{\mathbf{k}\in\Omega^*} E_1(\mathbf{k}) = E_1(\mathbf{0})$, and $E_1(\mathbf{k})$ is non degenerate near the origin with a positive definite Hessian matrix (see e.g. [28]). The same reference insures the existence of the following quadratic expansion of $E_1(\mathbf{k})$ for $\mathbf{k} \to \mathbf{0}$:

$$E_1(\mathbf{k}) = E_0 + \frac{1}{2!}\mathbf{k}^T \left[\frac{\partial^2 E_1}{\partial k_i \partial k_j}(\mathbf{0})\right]_{1\leq i,j\leq 3} \mathbf{k} + \mathcal{O}\left(\mathbf{k}^4\right) \quad \text{when } \mathbf{k} \to 0$$

As the Hessian matrix is symmetric, then up to a change of coordinates this quadratic expansion can be rewritten as:

$$E_1(\mathbf{k}) = E_0 + \frac{1}{2}\sum_{i=1}^{3} \frac{k_i^2}{m_i^*} + \mathcal{O}\left(\mathbf{k}^4\right) \quad \text{when } \mathbf{k} \to 0 \tag{5.1}$$

where $\left[\frac{1}{m_i^*}\right]_{1\leq i\leq 3}$ are the eigenvalues of the inverse effective-mass tensor.

Consider the assumption of weak density $\rho_0 \in (0, 1)$. In this case the Fermi energy defined by (1.12) lies in the interval $(E_0, \max_{\mathbf{k}\in\Omega^*} E_1(\mathbf{k}))$. When $\rho_0 \to 0$ it follows that $\mathcal{E}_F(\rho_0)$ converges to E_0. The $\mathbf{k}$-subset of Ω^* where $E_0 \leq E_1(\mathbf{k}) \leq \mathcal{E}_F(\rho_0)$ is therefore only localized near the origin.

From (5.1) we get the following asymptotic expansion of $\mathcal{E}_F(\rho_0) - E_0$ when $\rho_0 \to 0$ (the proof is given in the appendix of this section):

Proposition 5.1. *When $\rho_0 \to 0$, we have the following expansion*:

$$\mathcal{E}_F(\rho_0) - E_0 = s\rho_0^{\frac{2}{3}} + \mathcal{O}\left(\rho_0^{\frac{4}{3}}\right), \qquad s := \frac{(6\pi^2)^{\frac{2}{3}}}{2}\left(\frac{1}{m_1^* m_2^* m_3^*}\right)^{\frac{1}{3}}. \tag{5.2}$$

In the particular case when $m_i^* = m^* > 0$ for $i \in \{1, 2, 3\}$ and by setting $k_F := (6\pi^2\rho_0)^{\frac{1}{3}}$:

$$\mathcal{E}_F(\rho_0) - E_0 = \frac{1}{2m^*}k_F^2 + \mathcal{O}\left(k_F^4\right). \tag{5.3}$$

Before proving Theorem 1.2 (iii), we need one more technical result (its proof is also in the appendix of this section):

Lemma 5.2. *Assume that $E_1(\mathbf{k})$ remains non-degenerate on the ball $B_{\epsilon_0}(\mathbf{0}) := \{\mathbf{k} \in \Omega^* : |\mathbf{k}| \leq \epsilon_0\}$ with $\epsilon_0 > 0$ small enough. Consider any continuous function $F : B_{\epsilon_0}(\mathbf{0}) \to \mathbb{C}$. Then when $\rho_0 \to 0$ we have the following asymptotic expansions*:

$$\int_{\mathcal{S}_F} \frac{\mathrm{d}\sigma(\mathbf{k})}{|\nabla E_1(\mathbf{k})|} F(\mathbf{k}) = A\rho_0^{\frac{1}{3}} + o\left(\rho_0^{\frac{1}{3}}\right) \quad \textit{with} \quad A := \sqrt{m_1^* m_2^* m_3^*}\, 4\sqrt{2}\pi F(\mathbf{0})\sqrt{s} \tag{5.4}$$

and

$$\int_{\Omega^*} \mathrm{d}\mathbf{k}\, \chi_{[E_0, \mathcal{E}_F(\rho_0)]}\left(E_1(\mathbf{k})\right) F(\mathbf{k}) = B\rho_0 + o\left(\rho_0\right)$$

$$\text{with} \quad B := \sqrt{m_1^* m_2^* m_3^*} \frac{8\sqrt{2}\pi}{3} F(\mathbf{0}) s^{\frac{3}{2}}, \tag{5.5}$$

where s is the coefficient defined in (5.2).

Now we are ready to prove the Landau-Peierls formula in (1.17). For this, consider the formula (1.16). Remember that $E_1(\cdot)$ is non-degenerate and analytic in a neighborhood of the origin. Let us concentrate ourselves on the first term appearing in (1.16):

$$-\left(\frac{\mathrm{e}}{c}\right)^2 \frac{1}{12} \frac{1}{(2\pi)^3} \int_{\mathcal{S}_F} \frac{\mathrm{d}\sigma(\mathbf{k})}{|\nabla E_1(\mathbf{k})|} \times \left\{ \frac{\partial^2 E_1(\mathbf{k})}{\partial k_1^2} \frac{\partial^2 E_1(\mathbf{k})}{\partial k_2^2} - \left(\frac{\partial^2 E_1(\mathbf{k})}{\partial k_1 \partial k_2} \right)^2 - 3\mathcal{F}_1(\mathbf{k}) \right\}, \tag{5.6}$$

since only this term will have a nonzero contribution to the leading term in (1.17). The other term will go to zero like ρ_0; this can be shown using (5.5), (5.1), and the fact that the coefficients $\mathfrak{c}_{1,1}$ and $\mathfrak{c}_{1,0}$ are continuous near $\mathbf{0}$ (see Lemma 3.7).

Now consider the following function:

$$F(\mathbf{k}) := \frac{\partial^2 E_1(\mathbf{k})}{\partial k_1^2} \frac{\partial^2 E_1(\mathbf{k})}{\partial k_2^2} - \left(\frac{\partial^2 E_1(\mathbf{k})}{\partial k_1 \partial k_2} \right)^2 - 3\mathcal{F}_1(\mathbf{k}).$$

By taking into account that $\mathcal{F}_1(\cdot) = -2\mathfrak{a}_{1,2}(\cdot)$ (see (4.11)) and by virtue of Lemma 3.7, $F(\cdot)$ is continuous near the origin. According to (5.4), the only thing we need to do is to compute $F(\mathbf{0})$. The determinant of the Hessian matrix gives after a short computation:

$$\frac{\partial^2 E_1(\mathbf{k})}{\partial k_1^2} \frac{\partial^2 E_1(\mathbf{k})}{\partial k_2^2} - \left(\frac{\partial^2 E_1(\mathbf{k})}{\partial k_1 \partial k_2} \right)^2 = \frac{1}{m_1^* m_2^*} + \mathcal{O}\left(\mathbf{k}^2\right) \quad \text{when } \mathbf{k} \to \mathbf{0}. \tag{5.7}$$

Thus we can write:

$$\mathcal{X}_{\mathrm{M}}(\rho_0) = -\left(\frac{\mathrm{e}}{c}\right)^2 \frac{1}{24\pi^2} \left(m_1^* m_2^* m_3^*\right)^{\frac{1}{3}} \left[\frac{1}{m_1^* m_2^*} - 3\mathcal{F}_1(\mathbf{0}) \right] (6\pi)^{\frac{1}{3}} \rho_0^{\frac{1}{3}} + o\left(\rho_0^{\frac{1}{3}}\right) \quad \text{when } \rho_0 \to 0.$$

The only thing we have left to do, is proving that $\mathcal{F}_1(\mathbf{0}) = 0$. The definition of $\mathcal{F}_1$ can be found in (4.11), while the coefficients entering in its definition are defined in (3.29).

Let us start by showing that for all integers $j_2, j_3 \geq 2$ we have:

$$\mathcal{C}_{1,1,j_2,j_3}(\mathbf{0}) = \mathcal{C}_{1,j_2,j_3,1}(\mathbf{0}) = \mathcal{C}_{j_2,1,1,1}(\mathbf{0}) = \mathcal{C}_{1,1,j_2,1}(\mathbf{0}) = 0.$$

Indeed, in the expression of each of these functions it is possible to identify a factor of the type $\hat{\pi}_{1,1}(\alpha; \mathbf{0}), \alpha \in \{1, 2\}$ which are nothing but partial derivatives of E_1 at the origin, thus they must be zero. It follows that:

$$\mathcal{F}_1(\mathbf{0}) = \sum_{j_2=2}^{\infty} \sum_{j_3=2}^{\infty} \frac{\mathcal{C}_{1,j_2,1,j_3}(\mathbf{0})}{(E_{j_2}(\mathbf{0}) - E_1(\mathbf{0}))\,(E_{j_3}(\mathbf{0}) - E_1(\mathbf{0}))}. \tag{5.8}$$

Since:

$$\begin{aligned}\mathcal{C}_{1,j_2,1,j_3}(\mathbf{0}) = & \hat{\pi}_{1,j_2}(1;\mathbf{0})\hat{\pi}_{j_2,1}(2;\mathbf{0})\hat{\pi}_{1,j_3}(2;\mathbf{0})\hat{\pi}_{j_3,1}(1;\mathbf{0}) \\ & +\hat{\pi}_{1,j_2}(2;\mathbf{0})\hat{\pi}_{j_2,1}(1;\mathbf{0})\hat{\pi}_{1,j_3}(1;\mathbf{0})\hat{\pi}_{j_3,1}(2;\mathbf{0}) \\ & -\hat{\pi}_{1,j_2}(2;\mathbf{0})\hat{\pi}_{j_2,1}(1;\mathbf{0})\hat{\pi}_{1,j_3}(2;\mathbf{0})\hat{\pi}_{j_3,1}(1;\mathbf{0}) \\ & -\hat{\pi}_{1,j_2}(1;\mathbf{0})\hat{\pi}_{j_2,1}(2;\mathbf{0})\hat{\pi}_{1,j_3}(1;\mathbf{0})\hat{\pi}_{j_3,1}(2;\mathbf{0}),\end{aligned}$$

then (5.8) can be rewritten as :

$$\begin{aligned}\mathcal{F}_1(\mathbf{0}) = 2\left|\sum_{j=2}^{\infty}\frac{\hat{\pi}_{1,j}(2;\mathbf{0})\hat{\pi}_{j,1}(1;\mathbf{0})}{E_j(\mathbf{0})-E_1(\mathbf{0})}\right|^2 - \left(\sum_{j=2}^{\infty}\frac{\hat{\pi}_{1,j}(2;\mathbf{0})\hat{\pi}_{j,1}(1;\mathbf{0})}{E_j(\mathbf{0})-E_1(\mathbf{0})}\right)^2 \\ - \left(\overline{\sum_{j=2}^{\infty}\frac{\hat{\pi}_{1,j}(2;\mathbf{0})\hat{\pi}_{j,1}(1;\mathbf{0})}{E_j(\mathbf{0})-E_1(\mathbf{0})}}\right)^2 .\end{aligned} \tag{5.9}$$

But for $\mathbf{k}=0$ we may choose all our eigenfunctions $u_l(\cdot\,;\mathbf{0})$ to be real. It means that for all integers $j \geq 2$ and $\alpha \in \{1,2\}$, the matrix elements $\hat{\pi}_{1,j}(\alpha;\mathbf{0})$ are purely imaginary. As a result, the sums in (5.9) are real numbers and cancel each other, thus $\mathcal{F}_1(\mathbf{0}) = 0$. □

5.2. Appendix—Proofs of Intermediate Results

Here we prove Proposition 5.1 and Lemma 5.2.

Proof of Proposition 5.1. In (5.1) use the change of variables $\tilde{k}_i := \frac{k_i}{\sqrt{m_i^*}}$, with $i \in \{1,2,3\}$. This gives:

$$\tilde{E}_1(\tilde{\mathbf{k}}) := E_1(\sqrt{m_i^*}\,\tilde{\mathbf{k}}) = E_0 + \frac{1}{2}\left\{\tilde{k}_1^2 + \tilde{k}_2^2 + \tilde{k}_3^2\right\} + \mathcal{O}(\tilde{\mathbf{k}}^4).$$

In spherical coordinates:

$$\tilde{E}_1(r,\theta,\phi) = E_0 + \frac{1}{2}r^2 + \mathcal{O}(r^4) \quad \text{when } r \to 0. \tag{5.10}$$

We would like to express r as a function of $\tilde{E}_1, \theta$ and ϕ. Clearly, the equation $\tilde{E}_1\left(r(\theta,\phi),\theta,\phi\right) = E_0 + \Delta$ has a unique solution $r(\theta,\phi,\Delta)$ if $\Delta > 0$ is small enough. This solution obeys a fixed point equation of the type:

$$r(\theta,\phi,\Delta) = \sqrt{2\Delta}\left[1 + \mathcal{O}\left(r^2(\theta,\phi,\Delta)\right)\right] \tag{5.11}$$

which leads to the estimate:

$$r(\theta,\phi,\Delta) = \sqrt{2\Delta}\left[1 + \mathcal{O}\left(\Delta\right)\right] \quad \text{when } \Delta \to 0. \tag{5.12}$$

We can finally determine Δ (thus the Fermi energy) as a function ρ_0. By setting $\tilde{\Omega}^* := \frac{\Omega^*}{\sqrt{m_1^* m_2^* m_3^*}}$, it follows from (2.6):

$$\rho_0 = \frac{\sqrt{m_1^* m_2^* m_3^*}}{(2\pi)^3}\int_{\tilde{\Omega}^*} \mathrm{d}\tilde{\mathbf{k}}\,\chi_{[E_0,E_0+\Delta]}\left(\tilde{E}_1(\tilde{\mathbf{k}})\right).$$

Using spherical coordinates:

$$\rho_0 = \frac{\sqrt{m_1^* m_2^* m_3^*}}{(2\pi)^3} \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin\theta \left\{ \int_0^{\sqrt{2\Delta}} \mathrm{d}r \, r^2 + \int_{\sqrt{2\Delta}}^{r(\theta,\phi,\Delta)} \mathrm{d}r \, r^2 \right\}.$$

This is the equation we have to solve in order to find Δ as a function of ρ_0. Then by standard fixed point arguments we arrive at the estimate (5.2) and we are done. □

Proof of Lemma 5.2. We only prove (5.4), the other estimate being similar. As before, we prefer the new variables $\tilde{k}_i = \frac{k_i}{\sqrt{m_i^*}}$ where $i \in \{1,2,3\}$. Denote by $\tilde{E}_1(\tilde{\mathbf{k}}) = E_1(\mathbf{k})$, by $\tilde{F}(\tilde{\mathbf{k}}) = F(\mathbf{k})$ and with $\tilde{\Omega}^* := \frac{\Omega^*}{\sqrt{m_1^* m_2^* m_3^*}}$. Then we can formally write:

$$\begin{aligned}
\int_{\mathcal{S}_F} \frac{\mathrm{d}\sigma(\mathbf{k})}{|\nabla E_1(\mathbf{k})|} F(\mathbf{k}) &= \int_{\Omega^*} \mathrm{d}\mathbf{k} \, \delta\left(\mathcal{E}_F(\rho_0) - E_1(\mathbf{k})\right) F(\mathbf{k}) \\
&= \sqrt{m_1^* m_2^* m_3^*} \int_{\tilde{\Omega}^*} \mathrm{d}\tilde{\mathbf{k}} \, \delta\left(\mathcal{E}_F(\rho_0) - \tilde{E}_1(\tilde{\mathbf{k}})\right) \tilde{F}(\tilde{\mathbf{k}}) \\
&= \sqrt{m_1^* m_2^* m_3^*} \int_{\{\tilde{\mathbf{k}} \in \tilde{\Omega}^* \text{ s.t. } \tilde{E}_1(\tilde{\mathbf{k}}) = \mathcal{E}_F(\rho_0)\}} \frac{\mathrm{d}\sigma(\tilde{\mathbf{k}})}{|\nabla_{\tilde{\mathbf{k}}} \tilde{E}_1(\tilde{\mathbf{k}})|} \tilde{F}(\tilde{\mathbf{k}}).
\end{aligned} \tag{5.13}$$

The quadratic expansion (5.1) implies $|\nabla_{\tilde{\mathbf{k}}} \tilde{E}_1(\tilde{\mathbf{k}})| = |\tilde{\mathbf{k}}| \left[1 + \mathcal{O}\left(\tilde{\mathbf{k}}^2\right)\right]$ when $\tilde{\mathbf{k}} \to \mathbf{0}$. Then:

$$\begin{aligned}
&\int_{\mathcal{S}_F} \frac{\mathrm{d}\sigma(\mathbf{k})}{|\nabla E_1(\mathbf{k})|} F(\mathbf{k}) \\
&\quad = \sqrt{m_1^* m_2^* m_3^*} F(\mathbf{0}) \int_{\{\tilde{\mathbf{k}} \in \tilde{\Omega}^* \text{ s.t. } \tilde{E}_1(\tilde{\mathbf{k}}) = \mathcal{E}_F(\rho_0)\}} \mathrm{d}\sigma(\tilde{\mathbf{k}}) \, |\tilde{\mathbf{k}}|^{-1} \left[1 + o(1)\right].
\end{aligned} \tag{5.14}$$

Using spherical coordinates, let us denote as before by $r(\theta,\phi,\rho_0)$ the unique root of the equation $\tilde{E}_1\left(r(\theta,\phi,\rho_0),\theta,\phi\right) = \mathcal{E}_F(\rho_0)$. Then (5.14) can be rewritten as:

$$\begin{aligned}
&\int_{\mathcal{S}_F} \frac{\mathrm{d}\sigma(\mathbf{k})}{|\nabla E_1(\mathbf{k})|} F(\mathbf{k}) \\
&\quad = \sqrt{m_1^* m_2^* m_3^*} F(\mathbf{0}) \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \mathrm{d}\theta \, \sin(\theta) \, r(\theta,\phi,\rho_0) \left[1 + o(1)\right].
\end{aligned}$$

Now by setting $\Delta := \mathcal{E}_F(\rho_0) - E_0$ and by using (5.12) when $\Delta \to 0$:

$$\int\limits_{\mathcal{S}_F} \frac{\mathrm{d}\sigma(\mathbf{k})}{\left|\nabla E_1(\mathbf{k})\right|} F(\mathbf{k}) = \sqrt{m_1^* m_2^* m_3^*}\, 4\sqrt{2}\pi F(\mathbf{0})\, \sqrt{\Delta}\,[1 + o(1)]\,.$$

Finally, we use (5.2) and the proof is over. □

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