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Number of States and the Magnetic Properties of an Electron Gas

A. W. SÁENZ AND R. C. O'ROURKE

*Radiation Division, Naval Research Laboratory, Washington 25, D. C.**

INTRODUCTION

THE problem of deriving the thermodynamic properties of conduction electrons in metals can be reduced to that of computing the number of states $N(E)$ with energy less than E for the case of interest. The primary purpose of this paper is the present methods for calculating $N(E)$. Its secondary purpose is to apply these methods to various problems in the theory of metals and in particular to the case of electrons in a magnetic field.

Before outlining the contents of the present paper, we shall sketch the historical background of the methods discussed in the following pages.

The problem of computing $N(E)$ for systems composed of identical and noninteracting parts can be reduced to that of calculating traces of certain exponential operators. This last problem is formally identical to the evaluation of the partition function in quantum statistics (see Sec. 1.1).

The first author to recognize and exploit this fact was Peierls,[1] in connection with the magnetic properties of conduction electrons in metals. The main advantage of computing $N(E)$ in terms of traces is that one need not have any knowledge of the eigenfunctions and eigenvalues of the Hamiltonian of the system of interest. The recent work of Sondheimer and Wilson[2] on the magnetic properties of free electrons is based on ideas of this type. An important contribution of this paper is the fact that powerful complex variable techniques are introduced for evaluating $N(E)$ in terms of traces of exponential operators.

Perturbation-theoretic methods for calculating such traces for systems so complicated that it would be out of the question to evaluate them exactly have been developed by many workers in the quantum-statistical theory of nonideal gases and the theory of metals.

In the first category, the papers of Kirkwood,[3] Uhlenbeck and Beth,[4] and Goldberger and Adams[5] are basic for our present purposes. Reference 5 is particularly relevant, because it introduces a modern way for performing trace computations, inspired by a procedure of Schwinger[6] in quantum electrodynamics. Method I of our article is based on certain results of reference 5 (see Sec. 1.2).

In the second category, we mention the beautiful study of Peierls[1] alluded to earlier, which contains a procedure for calculating traces of exponential operators which is related in a formal manner to the work in references 3, 4, and 5, and to our Method II (see Sec. 1.2).

The most important application of the foregoing methods, as far as the present paper is concerned, is to the study of the magnetic properties of metals. A complete historical and critical summary of the older papers on the subject up to the year 1931 is contained in the excellent text of Van Vleck.[7] The more modern aspects of the problem can be found in numerous publications, such as Sondheimer and Wilson,[2] Dingle,[8] Osborne and Steele.[9] More specific references, as well as the relation of the calculational procedures used in previous work to our own, will be given in the body of this paper (see Sec. 2.4).

We shall now give an outline of the present article.

In Sec. 1.1 we employ arguments essentially due to Dingle[8] to reduce the problem of computing $N(E)$ to that of evaluating $\mathfrak{N}(E)$, the number of orbital states with energy less than E, thus eliminating the difficulties introduced by the spin from future calculations. The problem of obtaining $\mathfrak{N}(E)$ is virtually solved if we can calculate traces of suitable exponential operators, involving the spin-independent Hamiltonian $\mathfrak{H}$ [see Eq. (1.1.6)], as would be expected in view of our earlier remarks.

In Sec. 1.2 we present two methods for evaluating such traces. Method I rests on the so-called Schwinger trace formula [see Eq. (1.2.8)], stated in the paper of Goldberger and Adams.[6] Method II is based on a procedure for expanding exponential operators similar to those in references 1, 4, and 5. We show that Method II is better than Method I in the sense that the Nth approximation in Method I is *properly* contained in the corresponding Nth approximation in Method II. As far as practical applications are concerned, there are

* One of the authors (A.W.S.) was in the Applied Mathematics Branch, Mechanics Division, Naval Research Laboratory, during a major portion of the time required to complete this paper.

[1] R. Peierls, Z. Physik **80**, 763 (1933).

[2] E. H. Sondheimer and A. H. Wilson, Proc. Roy. Soc. (London) **A270**, 173 (1951).

[3] See the excellent review of J. de Boer, Repts. Progr. in Phys. **12**, 305 (1948–1949) for complete references on the work of J. G. Kirkwood in quantum statistics.

[4] G. Uhlenbeck and E. Beth, Physica **3**, 729 (1936).

[5] M. L. Goldberger and E. N. Adams, II, J. Chem. Phys. **20**, 240 (1952).

[6] J. Schwinger, Phys. Rev. **82**, 664 (1951), Sec. VI.

[7] Van Vleck, *Electric and Magnetic Susceptibilities* (Oxford University Press, London, 1932), first edition.

[8] R. B. Dingle, Proc. Roy. Soc. (London) **A211**, 500 (1952).

[9] M. F. M. Osborne, Phys. Rev. **88**, 438 (1952); M. C. Steele, Phys. Rev. **88**, 451 (1952).

important differences between I and II. The main difference is that I appears to be particularly suitable for the discussion of properties of weakly bound electrons, while II would seem to be applicable not only to this situation, but also to the case when the perturbing potentials are slowly varying over certain microscopic intervals, but are not necessarily "small" compared to the kinetic energy of the particles of the system of interest.

In Sec. 1.3, using I and II, we present asymptotic formulas for calculating the number of states for systems confined to the interior of "large" containers. In this discussion, the notion of wall potential plays a central role. The advantage of dealing with such large systems is that $\mathfrak{N}(E)$, and thus $N(E)$, can be replaced by smooth functions of E.

In Sec. 1.4 we formulate the problem of calculating the magnetic moment of an electron gas in a periodic potential supposing that the system is in a large container, in the sense of inequality (2.2.1). We find that the free energy, thermodynamic potential, and, *a fortiori*, the magnetic moment, have the correct dependence on the volume of the container.

In Part 2, we apply the foregoing methods to two examples.

In Sec. 2.1 we use Method I to calculate $N(E)$ for weakly bound electrons in a periodic potential to within terms with $n\leqslant 2$ in the sense of Eq. (1.3.15).

In Sec. 2.2 we compute $N(E)$ for a gas of free electrons in a magnetic field and discuss the corresponding magnetic moment. This case is one of the few problems in quantum statistics where an exact solution can be found, and a great deal of attention has been given to it, as can be seen from the number of references in Van Vleck[7] and in Sec. 2.2. The basic tool which we employ in obtaining $N(E)$ is a celebrated formula due to Mehler and applied very early to quantum-statistical problems by Uhlenbeck[10] and Husimi.[11] We believe that our approach, although yielding no new results, represents a fresh and simple way of discussing this question.

It would be most interesting to treat the effect of the walls on the magnetic properties of free electrons by means of Method II. We hope that the procedures presented here will be of aid in solving the difficult problem of the magnetic properties of electrons in periodic potentials.

In the Appendix we present a proof of Eq. (1.2.9), which is virtually the Schwinger trace formula, for terms with $n\leqslant 2$. In this proof we employ only elementary results from degenerate perturbation theory.

In this paper we are chiefly concerned with obtaining formal results. We do not investigate questions of convergence or the legitimacy of interchanging limiting processes. However, we have been very careful to point out such interchanges when they occur. The mathematical problems left open are fascinating ones in their own right and we hope that they will stimulate the attention which they deserve.

[10] G. E. Uhlenbeck, J. Math. and Phys. **14**, 10 (1935). A proof of the Mehler formula may be found in A. Erdélyi, Math. Z. **44**, 201 (1938).

[11] K. Husimi, Proc. Phys. Math. Soc. Japan **22**, 264 (1940).

PART 1: GENERAL METHODS

1.1. General Relations between $N(E)$ and Traces of Exponential Operators

In the present paper, we shall deal with systems composed of a large number of identical parts, whose mutual interactions we shall suppose to be negligible. Because of this circumstance, their total Hamiltonians are equal to a sum of identical one-particle Hamiltonians. We shall suppose that the latter possess pure point spectra, that the degeneracy of the energy eigenvalues is finite, and that there is a minimum eigenvalue. In discussing the statistical-mechanical theory of such assemblies, we shall encounter sums of the types

$$S=\sum_p F(E_p), \tag{1.1.1}$$

involving the values of functions $F(E)$ at the eigenvalues E_p of one of the aforementioned one-particle Hamiltonians, say $\mathfrak{H}_T$.[12,13] In (1.1.1), p specifies a one-particle state of the system and the sum runs over *all* these states.

The evaluation of such sums is greatly facilitated by the introduction of function $N(E)$ defined as

$$N(E)\equiv\sum_p U(E-E_p), \tag{1.1.2}$$

where

$$U(x)\equiv\begin{cases}0 & x<0,\\ \frac{1}{2} & x=0,\\ 1 & x>0.\end{cases} \tag{1.1.3}$$

From (1.1.2) we can interpret $N(E)$ as the number of states with energy smaller than E, provided that E does not coincide with any of the E_p.

Let $F(E)$ be differentiable in E, and let it vanish for $E\rightarrow\infty$. Then

$$S=-\int_{-\infty}^{\infty}dE\frac{dF(E)}{dE}N(E), \tag{1.1.1$'$}$$

as the following argument shows:

$$-\int_{-\infty}^{\infty}dE\frac{dF(E)}{dE}N(E)=-\int_{-\infty}^{\infty}dE\frac{dF(E)}{dE}\sum_p U(E-E_p)$$
$$=-\sum_p\int_{E_p}^{\infty}dE\frac{dF(E)}{dE}=\sum_p F(E_p).$$

[12] It will not be necessary to use an index to denote the particular one-particle Hamiltonian we are considering since only their structure plays a role in this paper and since this structure is common to all of them.

[13] In this article, we shall always denote abstract operators by lightface or boldface German letters, depending on whether we are dealing with scalars or vectors. We shall designate the eigen-

We shall now exploit the fact that $U(x)$ has the following integral representation[14]:

$$U(x)=\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{dz}{z}e^{zx}, \tag{1.1.3$'$}$$

where

$$\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\equiv\lim_{T\to\infty}\int_{\gamma-iT}^{\gamma+iT}dz.$$

We suppose that the series

$$\sum_p \exp(-zE_p)=\text{trace}\exp(-z\mathfrak{H}_T), \tag{1.1.4}$$

where we employ the familiar trace notation, converges for $\text{Re}\{z\}>0$, and furthermore, that we can interchange $\sum_p$ and

$$\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz$$

in what follows. From (1.1.2), (1.1.3)′, and (1.1.4), we are then led to the identity[15]

$$N(E)=\mathcal{P}\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}\text{trace}\exp(-z\mathfrak{H}_T). \tag{1.1.5}$$

Now, $\text{trace}\exp(-z\mathfrak{H}_T)$ is nothing more than the analytic continuation of the ordinary partition function

$$Z(\beta)\equiv\text{trace}\exp(-\beta\mathfrak{H}_T)=\sum_p\exp(-\beta E_p),\quad \beta\equiv 1/kT, \tag{1.1.4$'$}$$

in the sense that we have replaced β by the complex variable z, whose real part is positive.

In the present paper, we shall deal with Hamiltonians which can be separated into two commuting parts $\mathfrak{H}$ and $\mathfrak{H}_s$, where $\mathfrak{H}$ stands for an orbital and $\mathfrak{H}_s$ for a spin Hamiltonian, so that

$$\mathfrak{H}_T=\mathfrak{H}+\mathfrak{H}_s;\quad \mathfrak{H}\mathfrak{H}_s=\mathfrak{H}_s\mathfrak{H}. \tag{1.1.6}$$

The eigenvalues E_p are therefore separable into a part E_n belonging to $\mathfrak{H}$ and $g\hbar\omega m$ belonging to $\mathfrak{H}_s$, where m takes all integral or half-integral values from $-j$ to $+j$, depending on whether j is integral or half-integral, ω is the Larmor frequency $eH/2m_0c$, and g is the Lande factor, which is 2 for electrons. Therefore,

$$E_p=E_n+g\hbar\omega m;\quad |m|\leqslant j;\quad j=0,\tfrac{1}{2},1,\cdots. \tag{1.1.7}$$

Since the eigenvalues E_p of $\mathfrak{H}_T$ are purely discrete, so are the eigenvalues E_n of $\mathfrak{H}$.

values of these operators by the corresponding Latin lightface or boldface letters. We shall not employ any fixed symbolism for eigenoperators.

[14] See, for example, G. Doetsch, *Theorie und Anwendung der Laplace-Transformation* (Dover Publications, New York, 1943), p. 105.

[15] The earliest application of formulas of this type to the theory of metals occurs in reference 2.

From (1.1.4), (1.1.6), and (1.1.7), we see that $\text{trace}\exp(-z\mathfrak{H}_T)$ is factorable:

$$\text{trace}\exp(-z\mathfrak{H}_T)=\text{trace}\exp(-z\mathfrak{H})\cdot\sum_{|m|\leqslant j}\exp(-zg\hbar\omega m), \tag{1.1.8}$$

$$\text{Re}\{z\}>0.$$

Combining (1.1.5) and (1.1.8), we arrive at the important formula[16]

$$N(E)=\sum_{|m|\leqslant j}\mathfrak{N}(E+g\hbar\omega m), \tag{1.1.9}$$

where

$$\mathfrak{N}(E)\equiv\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{\exp(zE)}{z}\text{trace}\exp(-z\mathfrak{H}).$$

This formula eliminates the difficulties introduced by the spin and reduces our problem to the computation of $\mathfrak{N}(E)$, which represents the number of orbital states with energy less than E, provided that E does not coincide with any of the E_n's. We shall show in the following pages that this problem is virtually solved if we can construct $\text{trace}\exp(-z\mathcal{H})$, since there exist powerful complex-variable methods for evaluating the contour integral in (1.1.9).

Consider now an arbitrary representation, say the λ-diagonal representation, whose states are supposed to be complete and orthonormal, so that we have, in particular,

$$\sum_n\langle\lambda'|n\rangle\langle n|\lambda\rangle=\delta(\lambda'-\lambda),\quad \int d\lambda\langle n'|\lambda\rangle\langle\lambda|n\rangle=\delta_{n',n}, \tag{1.1.10}$$

where we have assumed, for convenience in future discussions, that the λ's form a purely continuous spectrum.

It is now advantageous to introduce the density matrix

$$\langle\lambda'|\mathfrak{P}(z)|\lambda\rangle\equiv\sum_n\langle\lambda'|n\rangle\exp(-zE_n)\langle n|\lambda\rangle;\quad \text{Re}\{z\}>0, \tag{1.1.11}$$

where

$$\exp(\mathfrak{O})\equiv\sum_{n=0}^{\infty}\frac{1}{n!}\overbrace{\mathfrak{O}\cdot\mathfrak{O}\cdots\mathfrak{O}}^{n\text{ factors}}. \tag{1.1.12}$$

From now on we shall suppose $\text{Re}\{z\}>0$ and $\gamma>0$, without always stating this hypothesis explicitly.

Using (1.1.10) and (1.1.11), we find

$$\text{trace}\exp(-z\mathfrak{H})=\sum_n\exp(-zE_n)=\int d\lambda\langle\lambda|\mathfrak{P}(z)|\lambda\rangle. \tag{1.1.13}$$

[16] Compare with reference 8, especially p. 501.

It is well to emphasize the fact that in terms of the q-diagonal representation

$$\text{trace}\exp(-z\mathfrak{H})=\int_{-\infty}^{\infty}d\mathbf{q}'\langle\mathbf{q}'|\exp(-z\mathfrak{H})|\mathbf{q}'\rangle, \quad (1.1.13)'$$

where the integration extends over the entire configuration space.

The fact that the trace of an operator is invariant with respect to a change of basis is very welcome, since it means that we may employ any basis which is convenient for the problem at hand.

In the present study we shall identify the λ representation with the coordinate-diagonal representation and shall expand our results in terms of plane waves.

From (1.1.13), (1.1.13)′, and the fact that

$$\langle\mathbf{q}'|\exp(-z\mathfrak{H})|\mathbf{q}''\rangle =\exp\left[-z\mathfrak{H}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''},\mathbf{q}''\right)\right]\delta(\mathbf{q}'-\mathbf{q}'') \quad (1.1.14)$$

and

$$\delta(\mathbf{q}'-\mathbf{q}'')=(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp[-i\mathbf{k}\cdot(\mathbf{q}'-\mathbf{q}'')]$$

we conclude that

$$\langle\mathbf{q}'|\exp(-z\mathfrak{H})|\mathbf{q}''\rangle =(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}') \times\exp\left[-z\mathfrak{H}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''},\mathbf{q}''\right)\right]\exp(i\mathbf{k}\cdot\mathbf{q}''), \quad (1.1.15a)$$

$$\text{trace}\exp(-z\mathfrak{H}) =(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{q}'\int_{-\infty}^{\infty}d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}') \times\exp\left[-z\mathfrak{H}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}'},\mathbf{q}'\right)\right]\exp(i\mathbf{k}\cdot\mathbf{q}'). \quad (1.1.15b)$$

We shall call Eq. (1.1.15b) the Kirkwood-Uhlenbeck formula, since these authors were the first to recognize and exploit the advantages of plane wave bases in constructing partition functions in the theory of nonideal gases.[3–5]

Our further work rests on Eqs. (1.1.13), (1.1.13)′, and (1.1.15).

It is necessary to state at this point that the formal manipulations used in deriving these results cannot be justified for unrestricted operators $\mathfrak{H}$. Although the exact nature of the restrictions is unknown at present, it has been noted that one must be extremely careful with Hamiltonians whose coordinate dependence in the $\mathbf{q}'$-diagonal representation exhibits either finite or infinite discontinuities. The case of the rigid-sphere potential, for example, introduces complications of this type.[17]

In the following discussion, we shall deal only with Hamiltonians which are analytic functions of the coordinate and momentum operators, in an attempt to avoid the aforementioned pitfalls.

1.2. Two Methods for Calculating Traces of Exponential Operators

We are ready to consider two perturbation-theoretic methods for constructing trace$\{\exp(-z\mathfrak{H})\}$ for systems for which it would be out of the question to evaluate this trace exactly.

A. Method I

Let us begin with the simpler method, Method I. Consider the exponential operator

$$\mathfrak{Q}(s)\equiv\exp[-s(\mathfrak{a}+\mathfrak{b})], \quad (1.2.1)$$

where $\mathfrak{a}$ is "large" compared to $\mathfrak{b}$ in the conventional sense of perturbation calculus and s is a real parameter.

Following Goldberger and Adams, we define $\mathfrak{B}(s)$ as follows:

$$\mathfrak{Q}(s)\equiv\exp(-s\mathfrak{a})\mathfrak{B}(s). \quad (1.2.2)$$

Letting

$$\mathfrak{b}(s)\equiv\exp(s\mathfrak{a})\mathfrak{b}\exp(-s\mathfrak{a}), \quad (1.2.3)$$

we can conclude from (1.2.1) to (1.2.3) that $\mathfrak{B}(s)$ satisfies the initial value problem below:

$$\frac{\partial}{\partial s}\mathfrak{B}(s)=-\mathfrak{b}(s)\mathfrak{B}(s), \qquad \mathfrak{B}(0)=1, \quad (1.2.4)$$

where 1 is the unit operator.

Equations (1.2.4) are equivalent to the integral equation

$$\mathfrak{B}(s)=1-\int_0^s ds_1\mathfrak{b}(s_1)\mathfrak{B}(s_1), \quad (1.2.5)$$

whose formal solution, obtained by the usual iterative procedure, is

$$\mathfrak{B}(s)=\sum_{n=0}^{\infty}\mathfrak{B}_n(s), \qquad \mathfrak{B}_0(s)\equiv1, \qquad \mathfrak{B}_n(s)\equiv(-)^n\int_0^s ds_1\int_0^{s_1}ds_2\cdots \times\int_0^{s_{n-1}}ds_n\mathfrak{b}(s_1)\mathfrak{b}(s_2)\cdots\mathfrak{b}(s_n). \quad (1.2.6)$$

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[17] See, for example, G. V. Chester, Phys. Rev. 93, 606 (1952).

Combining (1.2.2) and (1.2.6), we obtain the formally exact identity

$$\mathfrak{Q}(s)=\exp(-s\mathfrak{a})\sum_{n=0}^{\infty}\mathfrak{V}_n(s). \quad (1.2.7)$$

It can be shown, from (1.2.6) and (1.2.7), that

$$\text{trace}\mathfrak{Q}(s)=\text{trace}\exp(-s\mathfrak{a})-\text{trace}\{\mathfrak{b}\exp(-s\mathfrak{a})\}$$
$$+\sum_{n=2}^{\infty}\frac{(-)^n}{n}\text{trace}\Big\{\mathfrak{b}\exp(-s\mathfrak{a})\int_0^s ds_1\int_0^{s_1}ds_2\cdots$$
$$\times\int_0^{s_{n-1}}ds_n\mathfrak{b}(s_1)\mathfrak{b}(s_2)\cdots\mathfrak{b}(s_n)\Big\}. \quad (1.2.8)$$

Goldberger and Adams[5,18] attribute this result to Schwinger. We shall call it the Schwinger trace formula.

A simple method of proving (1.2.8) for the case when $\mathfrak{a}$ has discrete eigenvalues is to calculate traces in the representation in which $\mathfrak{a}$ is diagonal.

Placing $s=1$; $\mathfrak{a}=z\mathfrak{H}_0$; $\mathfrak{b}=z\mathfrak{H}_1$, where $\mathfrak{H}_0$ is an unperturbed Hamiltonian and $\mathfrak{H}_1$ the corresponding perturbation operator, we get from (1.2.8)

$$\text{trace}\exp[-z(\mathfrak{H}_0+\mathfrak{H}_1)]=\text{trace}\exp(-z\mathfrak{H}_0)+\sum_{n=1}^{\infty}z^nF_n(z), \quad (1.2.9)$$

where

$$F_1(z)\equiv-\text{trace}\{\mathfrak{H}_1\exp(-z\mathfrak{H}_0)\},$$

$n\geqslant 2$:

$$F_n(z)\equiv\frac{(-)^n}{n}\text{trace}\Big\{\mathfrak{H}_1\exp(-z\mathfrak{H}_0)\int_0^{s_0=1}ds_1\int_0^{s_1}ds_2\cdots$$
$$\times\int_0^{s_{n-2}}ds_{n-1}\mathfrak{H}_1(s_1z)\mathfrak{H}_1(s_2z)\cdots\mathfrak{H}_1(s_nz)\Big\},$$

and

$$\mathfrak{H}_1(sz)\equiv\exp(-sz\mathfrak{H}_0)\mathfrak{H}_1\exp(sz\mathfrak{H}_0).$$

In the Appendix, we shall prove (1.2.9) for $n\leqslant 2$ by means of conventional degenerate perturbation theory.

The circumstance that the mth term of the sum in (1.2.9) contains $\mathfrak{H}_1$ *exactly* m times suggests that Method I is ideally suited to cases in which $\mathfrak{H}_1$ is "small" compared with $\mathfrak{H}_0$, in the usual sense of perturbation theory. We shall discuss a situation of this type in Sec. 2.1.

B. *Method II*

In this method, we begin by writing[19]

$$\mathfrak{Q}(s)=\exp(-s\mathfrak{b})\exp(-s\mathfrak{a})\mathfrak{W}(s). \quad (1.2.10)$$

From (1.2.10), we conclude that

$$\frac{\partial}{\partial s}\mathfrak{W}(s)=\mathfrak{T}(s)\mathfrak{W}(s), \quad (1.2.11)$$
$$\mathfrak{W}(0)=1,$$

where

$$\mathfrak{T}(s)\equiv\exp(s\mathfrak{a})\exp(s\mathfrak{b})[\exp(-s\mathfrak{b}),\mathfrak{a}]\times\exp(-s\mathfrak{a}), \quad (1.2.12)$$

where the square bracket represents a commutator.

In the cases considered in this paper, $\mathfrak{a}$ is quadratic and $\mathfrak{b}$ is at most linear in the one-particle momentum operator $\mathfrak{p}$, so that it is possible to work out the commutator in (1.1.30) in closed form. The final result does not involve exponential operators $\exp(\pm s\mathfrak{b})$. This result depends critically on the particular ordering of $\exp(-s\mathfrak{b})$ and $\exp(-s\mathfrak{a})$ in (1.2.10). For example, if this ordering were reversed, we would end up with commutators which could not be easily evaluated for the cases of interest.

Equations (1.2.11) are equivalent to the integral equation

$$\mathfrak{W}(s)=1+\int_0^s ds_1\mathfrak{T}(s_1)\mathfrak{W}(s_1), \quad (1.2.13)$$

whose formal solution, obtained by iteration, is thus

$$\mathfrak{W}(s)=\sum_{n=0}^{\infty}\mathfrak{W}_n(s), \quad (1.2.14)$$
$$\mathfrak{W}_0(s)\equiv 1,$$

$n\geqslant 1$:

$$\mathfrak{W}_n(s)\equiv\int_0^s ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{n-1}}ds_n\mathfrak{T}(s_1)\mathfrak{T}(s_2)\cdots\mathfrak{T}(s_n).$$

From (1.2.10) and (1.2.14), we obtain

$$\mathfrak{Q}(s)=\exp(-s\mathfrak{b})\exp(-s\mathfrak{a})\sum_{n=0}^{\infty}\mathfrak{W}_n(s). \quad (1.2.15)$$

We now show that the series (1.1.15) is better than (1.2.7) in the sense of the "dominance" theorem:

The Mth approximation,

$$\mathfrak{Q}_M{}^{(\mathrm{I})}(s)\equiv\exp(-s\mathfrak{a})\sum_{n=0}^{M}\mathfrak{V}_n(s), \quad (1.2.16a)$$

to $\mathfrak{Q}(s)$ *in Method I is properly contained in the Mth approximation*

$$\mathfrak{Q}_M{}^{(\mathrm{II})}(s)\equiv\exp(-s\mathfrak{b})\exp(-s\mathfrak{a})\sum_{n=0}^{M}\mathfrak{W}_n(s), \quad (1.2.16b)$$

to $\mathfrak{Q}(s)$ *in Method II, for* $M=0, 1, 2, \cdots$, *in the sense that all the terms of (1.2.16a) are contained in (1.2.16b) but not vice versa.*

[18] For another approach, see reference 17.

[19] This way of expanding exponential operators was employed by many of the early workers in quantum statistics, as can be see, for example, from reference 3. See also references 1 and 5 for expansion procedures of similar type.

Proof:

We shall prove this theorem for the nontrivial case[20] where $[\mathfrak{a},\mathfrak{b}]\neq 0$.

First, we observe that for $n=0, 1, 2, \cdots$ we have

$$\left.\begin{array}{l}\text{(i) } \exp(-s\mathfrak{a})\mathfrak{V}_n(s) \text{ contains only terms with exactly } n\mathfrak{b}\text{'s.}\\ \text{(ii) } \exp(-s\mathfrak{b})\exp(-s\mathfrak{a})\mathfrak{W}_n(s) \text{ contains an infinite number of terms with } r\mathfrak{b}\text{'s, } r\geqslant n, \text{ provided } [\mathfrak{a},\mathfrak{b}]\neq 0.\end{array}\right\} \quad (1.2.17)$$

Second, we notice that the expansions (1.2.7) and (1.2.15) represent the same operator $\mathfrak{Q}(s)$. Equating these expansions and using (1.2.16a) and (1.2.16b), we get:

$$\mathfrak{Q}_M{}^{(\mathrm{II})}(s)=\mathfrak{Q}_M{}^{(\mathrm{I})}(s)+\mathfrak{R}_M(s), \qquad (1.2.18)$$

where $\mathfrak{R}_M(s)$ contains solely terms with $\geqslant(M+1)\mathfrak{b}$'s $(M=0,1,2,\cdots)$.

Third, we employ (1.2.17), (1.2.18), and this property of $\mathfrak{R}_M(s)$ to deduce that all the terms of $\mathfrak{Q}_M{}^{(\mathrm{I})}(s)$ are contained in $\mathfrak{Q}_M{}^{(\mathrm{II})}(s)$, for $\mathfrak{R}_M(s)$ consists solely of terms having *more* than $M\mathfrak{b}$'s, while $\mathfrak{Q}_M{}^{(\mathrm{I})}(s)$ has only terms with $\leqslant M\mathfrak{b}$'s. On the other hand the terms of $\mathfrak{Q}_M{}^{(\mathrm{II})}(s)$ cannot all be contained in $\mathfrak{Q}_M{}^{(\mathrm{I})}(s)$ because, according to (1.2.16b) and (1.2.17), the former consists of a sum of terms with $r\mathfrak{b}$'s, where r takes on an *infinite* number of integral values $\geqslant M$, while $\mathfrak{Q}_M{}^{(\mathrm{I})}(s)$ consists of a *finite* number of terms each one of which contains $r\mathfrak{b}$'s, where $r\leqslant M$. *QED.*

Placing $s=1$; $\mathfrak{a}=z\mathfrak{H}_0$; $\mathfrak{b}=z\mathfrak{H}_1$, we obtain from (1.2.1), (1.2.14), and (1.2.15),

$$\operatorname{trace}\exp[-z(\mathfrak{H}_0+\mathfrak{H}_1)] =\operatorname{trace}\{\exp(-z\mathfrak{H}_1)\exp(-z\mathfrak{H}_0)\} +\sum_{n=1}^{\infty}z^nF_n'(z), \qquad (1.2.19)$$

where

$$F_n'(z)\equiv\operatorname{trace}\Big\{\exp(-z\mathfrak{H}_1)\exp(-z\mathfrak{H}_0) \times\int_0^1 ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{n-1}}ds_n \times\mathfrak{T}'(s_1z)\mathfrak{T}'(s_2z)\cdots\mathfrak{T}'(s_nz)\Big\},$$

and

$$\mathfrak{T}'(sz)\equiv\exp(sz\mathfrak{H}_0)\exp(sz\mathfrak{H}_1) \times[\exp(-sz\mathfrak{H}_1),\mathfrak{H}_0]\exp(-sz\mathfrak{H}_0).$$

In view of the preceding "dominance" theorem, we expect that the series (1.2.19) is more accurate than (1.2.9), if an equal number of terms is kept in both cases.

[20] If $[\mathfrak{a},\mathfrak{b}]=0$, Eqs. (1.2.12) and (1.1.14) imply that $\mathfrak{W}_n(s)=0$ for $n=1, 2, \cdots$, so that $\exp[-s(\mathfrak{a}+\mathfrak{b})]=\exp(-s\mathfrak{a})\exp(-s\mathfrak{b})$ as is well known.

It is clear that Method II is closely akin to the usual W. K. B. method of quantum mechanics. We thus expect that it will prove useful in cases where $\mathfrak{H}_1$, although not necessarily "small" compared to $\mathfrak{H}_0$, is nonetheless a slowly varying function of position in the $\mathbf{q}'$-diagonal representation over distances of the order of the mean De Broglie wavelength of the assembly of particles of interest.

1.3. $\mathfrak{N}(E)$ for Large Systems

The functions $\mathfrak{N}(E)$ in Sec. 1.1 are sums of step functions. The aim of the present section is to replace them by smooth functions of E for systems confined in containers which are "large" in a sense to be specified presently. The introduction of these smooth functions will enormously simplify the calculations in the succeeding sections. The results obtained below may be viewed as asymptotic expressions for containers whose volume $\Omega\rightarrow\infty$.

In carrying out this program, we shall make use of the concept of wall potential, whose main role is to simulate the walls of the aforementioned containers.

We now regard $\mathfrak{H}_0$ in Sec. 1.2 as composed of two parts:

$$\mathfrak{H}_0=\mathfrak{K}+\mathfrak{W}, \qquad (1.3.1a)$$

so that

$$\mathfrak{H}=\mathfrak{K}+\mathfrak{W}+\mathcal{H}_1, \qquad (1.3.1b)$$

where $\mathfrak{K}$ can represent, for example, the kinetic energy operator of a particle in Ω, while $\mathfrak{W}$ stands for the wall potential operator. $\mathfrak{W}$ depends only on $\mathbf{q}$ and its eigenvalues $W(\mathbf{q}')$, defined by

$$\mathfrak{W}(\mathfrak{q})|\mathbf{q}'\rangle=W(\mathbf{q}')|\mathbf{q}'\rangle \qquad (1.3.2)$$

are different from zero only when $\mathbf{q}'$ is close to the walls of Ω, in a sense which we proceed to make clear.

Figure 1 shows a sketch of the qualitative shape of which we shall adopt in this paper. The wall potential $W(\mathbf{q}')$ must effectively vanish in region I, which repre-

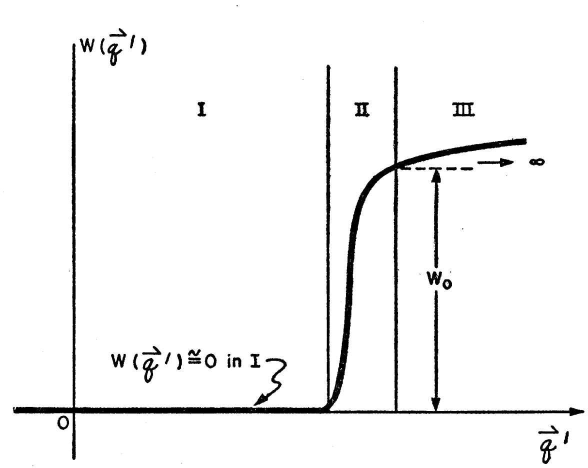

FIG. 1. Qualitative shape of $W(\mathbf{q}')$.

sents the interior of Ω. In II, which simulates the walls of Ω, $W(\mathbf{q}')$ must undergo an abrupt but continuous change to a large positive value W_0. In III, $W(\mathbf{q}')$ must go to infinity in any manner such that the wave functions $\langle n|\mathbf{q}'\rangle$, corresponding to the eigenvalues E_n of $\mathfrak{H}$, approach zero rapidly in this same region III. This particular choice of $W(\mathbf{q}')$ also eliminates the possibility of continuous spectra of $\mathfrak{H}$.

We shall now give a plausibility argument, based on the above model of $\mathfrak{W}$, for the validity of the formula below:

$$\int_{-\infty}^{\infty}d\mathbf{q}_1\int_{-\infty}^{\infty}d\mathbf{q}_2\cdots\int_{-\infty}^{\infty}d\mathbf{q}_r\mathfrak{F}(\mathbf{q}_1,\mathbf{q}_2,\cdots,\mathbf{q}_r)$$
$$\times\langle\mathbf{q}_1|\exp(-z\mathfrak{H})|\mathbf{q}_2\rangle\cdot\langle\mathbf{q}_2|\exp(-z\mathfrak{H})|\mathbf{q}_3\rangle\cdots$$
$$\times\langle\mathbf{q}_r|\exp(-z\mathfrak{H}|\mathbf{q}_1\rangle$$
$$\cong\int_{[\Omega]}d\mathbf{q}_1\int_{[\Omega]}d\mathbf{q}_2\cdots\int_{[\Omega]}d\mathbf{q}_r\mathfrak{F}(\mathbf{q}_1,\mathbf{q}_2,\cdots,\mathbf{q}_r)$$
$$\cdot\langle\mathbf{q}_1|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}_2\rangle$$
$$\times\langle\mathbf{q}_2|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}_3\rangle\cdots$$
$$\cdot\langle\mathbf{q}_r|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}_1\rangle,\qquad(1.3.3)$$

where $[\Omega]$ indicates an integration over Ω and where $\mathfrak{F}(\mathbf{q}_1,\cdots\mathbf{q}_r)$ is a smooth function of its arguments which is slowly varying over distances comparable to the thickness of the walls.

We shall base our arguments on Method II. It will be sufficient to consider the case $r=1$: the others can be dealt with similarly.

From (1.2.7), (1.2.12), (1.2.14), and (1.2.15), placing $\mathfrak{a}=z(\mathfrak{H}-\mathfrak{W})$; $\mathfrak{b}=z\mathfrak{W}$ we find:

$$\langle\mathbf{q}'|\exp(-z\mathfrak{H})|\mathbf{q}''\rangle=\exp[-zW(\mathbf{q}')]$$
$$\times\langle\mathbf{q}'|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}''\rangle$$
$$+\exp[-zW(\mathbf{q}')]\sum_{n=1}^{\infty}z^n\Bigg(\mathbf{q}'|\exp[-z(\mathfrak{H}-\mathfrak{W})]$$
$$\times\int_0^1ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{n-1}}ds_n\mathfrak{U}(s_1z)\mathfrak{U}(s_2z)\cdots$$
$$\times\mathfrak{U}(s_nz)|\mathbf{q}''\Bigg),\qquad(1.3.4)$$

where

$$\mathfrak{U}(sz)\equiv\exp[sz(\mathfrak{H}-\mathfrak{W})]\exp(sz\mathfrak{W})$$
$$\times[\exp(-sz\mathfrak{W}),\mathfrak{H}-\mathfrak{W}]\exp[-sz(\mathfrak{H}-\mathfrak{W})],$$

and where $\exp(sz\mathfrak{W})[\exp(-sz\mathfrak{W}),\mathfrak{H}-\mathfrak{W}]$ can be explicitly worked out in the coordinate diagonal representation for the Hamiltonian in (1.4.7), with the result

$$\langle\mathbf{q}'|\exp(sz\mathfrak{W})[\exp(-sz\mathfrak{W}),\mathfrak{H}-\mathfrak{W}]|\mathbf{q}''\rangle$$
$$=-\frac{\hbar^2}{2m}sz\Bigg\{\nabla_{\mathbf{q}'}{}^2W(\mathbf{q}')-sz(\nabla_{\mathbf{q}'}W(\mathbf{q}'))^2$$
$$+\frac{2ie}{\hbar c}\nabla_{\mathbf{q}'}W(\mathbf{q}')\cdot\mathbf{A}(\mathbf{q}')$$
$$+2\nabla_{\mathbf{q}'}W(\mathbf{q}')\cdot\nabla_{\mathbf{q}'}\Bigg\}\delta(\mathbf{q}''-\mathbf{q}').\qquad(1.3.5)$$

If the volume of region I, say Ω, is made arbitrarily large with respect to that of region II, keeping $W(\mathbf{q}')\cong0$ for $\mathbf{q}'$ in I and letting W_0 take on arbitrarily large values, we obtain, for *fixed* z and $\mathrm{Re}\{z\}>0$:

$$\int_{\infty}^{\infty}d\mathbf{q}'\mathfrak{F}(\mathbf{q}')\exp[-zW(\mathbf{q}')]$$
$$\times\langle\mathbf{q}'|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}'\rangle$$
$$\simeq\int_{[\Omega]}d\mathbf{q}'\mathfrak{F}(\mathbf{q}')\langle\mathbf{q}'|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}'\rangle.\qquad(1.3.6)$$

If it is possible, by an appropriate choice $W(\mathbf{q}')$ to dominate

$$\sum_{n=1}^{\infty}z^n\Bigg\langle\mathbf{q}'\Bigg|\exp[-z(\mathfrak{H}-\mathfrak{W})]\int_0^1ds_1\int_0^{s_1}sd_2\cdots\int_0^{s_{n-1}}ds_n$$
$$\cdot\mathfrak{T}'(s_1z)\mathfrak{T}'(s_2z)\cdots\mathfrak{T}'(s_nz)\Bigg|\mathbf{q}''\Bigg\rangle$$
$$\equiv P(\mathbf{q}',\mathbf{q}''|z),\qquad(1.3.7)$$

whose absolute value differs from zero only in regions II and III, by means of $\exp[-zW(\mathbf{q}')]$, in the sense of making the product of these quantities as small as desired, then we also have, for $\mathrm{Re}\{z\}>0$ and fixed z:

$$\int_{-\infty}^{\infty}d\mathbf{q}'\mathfrak{F}(\mathbf{q}')\exp[-zW(\mathbf{q}')]P(\mathbf{q}',\mathbf{q}''|z)\cong0.\qquad(1.3.8)$$

In view of the fact that each term of the sum (1.3.7) is a polynomial in $W(\mathbf{q}')$ and its derivatives, according to (1.3.5), its dominance by the exponential $\exp[-zW(\mathbf{q}')]$ in regions II and III is quite plausible.

If we accept (1.3.6) and (1.3.8), we arrive at the result (1.3.3) for $r=1$.

No attempt will be made to estimate the accuracy of (1.3.4) since the failure of this approximation would correspond to "surface phenomena." These phenomena are of importance only in small enough crystals. Criteria for determining whether a system is large in this sense are trustworthy if and only if they are based on actual calculations. A frequently used criterion for electrons in a magnetic field is given in Sec. 2.2.

From (1.3.3) follow two useful results.

First, we can combine this equation, for $n=1$ and $\mathfrak{F}(\mathbf{q}_1)=1$, with (1.1.9) and (1.1.13)′, thus obtaining

$$\mathfrak{N}(E)\cong\frac{1}{2\pi i}\int_{[\Omega]} d\mathbf{q}'\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{dz\exp(zE)}{z}\times\langle\mathbf{q}'|\exp[-z(\mathfrak{H}-\mathfrak{W})]|\mathbf{q}'\rangle. \quad (1.3.9)$$

The approximation (1.3.9) is valuable for the following reasons: the right-hand side can be calculated *without* knowing $\mathfrak{W}$ and is a smooth function of E for the case considered in detail in this paper (see Sec. 2.2); and it leads to interesting conclusions regarding the thermodynamic properties of the systems of interest (see Sec. 1.4).

Second, we can use (1.3.3) to construct a smooth function $\mathfrak{N}^*(E)$ to replace $\mathfrak{N}(E)$ by a perturbation method based on Methods I and II.

To carry out this construction, we use (1.1.13)′, (1.2.9), (1.3.1), and (1.3.3), where we replace $\mathfrak{H}$ by $\mathfrak{H}_0$, to reduce the integrations over configuration space to integrations over Ω. The replacement of $\mathfrak{H}$ by $\mathfrak{H}_0$ in (1.3.3) is legitimate, since it merely involves setting $\mathfrak{H}_1=0$ in this equation.

As an example, let us consider the first term on the right-hand side, employing the foregoing equations. We have

$$\begin{aligned}\text{trace}\exp(-z\mathfrak{H}_0)&=\text{trace}\exp[-z(\mathfrak{K}+\mathfrak{W})],\\ &=\int_{-\infty}^{\infty}d\mathbf{q}'\langle\mathbf{q}'|\exp[-z(\mathfrak{K}+\mathfrak{W})]|\mathbf{q}'\rangle,\\ &\cong\int_{[\Omega]}d\mathbf{q}'\langle\mathbf{q}'|\exp(-z\mathfrak{K})|\mathbf{q}'\rangle.\end{aligned}$$

Treating the remaining terms in a similar way, we obtain:

$$\text{trace}\exp(-z\mathfrak{H})\cong\int_{[\Omega]}d\mathbf{q}'\langle\mathbf{q}'|\exp(-z\mathfrak{K})|\mathbf{q}'\rangle+\sum_{n=1}^{\infty}z^nF_n^*(z),$$

$$F_1^*(z)\equiv-\int_{[\Omega]}d\mathbf{q}'\int_{[\Omega]}d\mathbf{q}_1\langle\mathbf{q}'|\mathfrak{H}_1|\mathbf{q}_1\rangle\langle\mathbf{q}_1|\exp(-z\mathfrak{K})|\mathbf{q}'\rangle,$$

$n\geqslant 2$:

$$\begin{aligned}F_n^*(z)=\frac{(-)^n}{n}\int_0^{s_0=1}ds_1\int_0^{s_1}ds_2\cdots\int_0^{s_{n-2}}ds_{n-1}&\times\int_{[\Omega]}d\mathbf{q}'\int_{[\Omega]}d\mathbf{q}_1\cdots\int_{[\Omega]}d\mathbf{q}_n\\ &\cdot\langle\mathbf{q}'|\mathfrak{H}_1|\mathbf{q}_1\rangle\langle\mathbf{q}_1|\exp(-z\mathfrak{K})|\mathbf{q}_2\rangle\\ &\times\langle\mathbf{q}_2|\mathfrak{H}_1^*(s_1z)|\mathbf{q}_3\rangle\cdots\\ &\times\langle\mathbf{q}_{n+1}|\mathfrak{H}_1^*(s_nz)|\mathbf{q}'\rangle,\end{aligned}\quad (1.3.10)$$

$$\langle\mathbf{q}_1|\mathfrak{H}^*(sz)|\mathbf{q}_2\rangle\equiv\int_{[\Omega]}d\mathbf{q}'\int_{[\Omega]}d\mathbf{q}''\langle\mathbf{q}_1|\exp(-sz\mathfrak{K})|\mathbf{q}'\rangle\cdot\langle\mathbf{q}'|\mathfrak{H}_1|\mathbf{q}''\rangle\langle\mathbf{q}''|\exp(-sz\mathfrak{K})|\mathbf{q}_2\rangle.$$

The expressions for $F_n^*(z)$ reduce to a much simpler form when $\mathfrak{H}_1$ is diagonal in the $\mathbf{q}'$-representation (see Sec. 2.1). In the case considered here, the $F_n^*(z)$ possess inverse Laplace transforms, and this will vastly simplify our further discussions.

The factors z^n in (1.1.42) require special care; otherwise they are bound to cause convergence difficulties. To overcome this obstacle, we begin by considering integrals of the type

$$\int_{-\infty}^{\infty}dEg(E)\mathfrak{N}(E),\quad\int_{-\infty}^{\infty}dE\left\{\int_{-\infty}^{E}dE'g(E')\right\}\mathfrak{N}(E),\quad (1.3.11)$$

where $g(E)$ has derivatives of all orders for $|E|<\infty$ and is negligible, together with its derivatives outside the interval

$$E_0-\epsilon\leqslant E\leqslant E_0+\epsilon,\quad (1.3.12)$$

where $\epsilon\ll E_0$. In the present paper, devoted to degenerate Fermi gases, we shall identify $g(E)$ with $(\partial/\partial E)f_0(E|\beta,\zeta)$ [see Eq. (1.4.8)′], which is very sharp in the vicinity of the Fermi energy $E=\zeta$ and has a half-width of order kT, so that we may choose $E_0\equiv\zeta$, $\epsilon\equiv kT$. We clearly have $\epsilon\ll E_0$, since $kT\ll\zeta$ for a degenerate Fermi gas.

We then write

$$\int_{-\infty}^{\infty}dEg(E)\mathfrak{N}(E)=\lim_{T\to\infty}\int_{-\infty}^{\infty}dEg(E)\frac{1}{2\pi i}\times\int_{\gamma-iT}^{\gamma+iT}dz\frac{\exp(zE)}{z}\cdot\text{trace}\exp(-z\mathfrak{H}),\quad (1.3.13)$$

interchanging the orders of

$$\lim_{T\to\infty}\quad\text{and}\quad\int_{-\infty}^{\infty}dE.$$

Combining (1.3.10) with (1.3.13), we obtain by partial integration, using the previously stated assumptions about $g(E)$,

$$\begin{aligned}\int_{-\infty}^{\infty}dEg(E)\mathfrak{N}(E)\cong&\lim_{T\to\infty}\int_{E_0-\epsilon}^{E_0+\epsilon}dEg(E)\cdot\frac{1}{2\pi i}\int_{\gamma-iT}^{\gamma+iT}dz\frac{\exp(zE)}{z}\int_{[\Omega]}d\mathbf{q}'\langle\mathbf{q}'|\exp(-z\mathfrak{H}_0)|\mathbf{q}'\rangle\\ &+\sum_{n=1}^{\infty}\lim_{T\to\infty}(-)^n\int_{E_0-\epsilon}^{E_0+\epsilon}dE\frac{\partial^ng(E)}{\partial E^n}\frac{1}{2\pi i}\times\int_{\gamma-iT}^{\gamma+iT}dz\frac{\exp(zE)}{z}F^{n*}(z),\end{aligned}$$

where we have interchanged

$$\sum_{n=1}^{\infty} \quad \text{and} \quad \lim_{T\to\infty} \int_{E_0-\epsilon}^{E_0+\epsilon} dE.$$

Taking $\lim_{T\to\infty}$ inside the integral and integrating partially once more, we get

$$\int_{-\infty}^{\infty} dE g(E)\mathfrak{N}(E) \simeq \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dE g(E)\mathfrak{N}_n{}^*(E),$$

$$\mathfrak{N}_0{}^*(E) \equiv \frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{\exp(zE)}{z} \times \int_{[\Omega]} d\mathbf{q}' \langle \mathbf{q}' | \exp(-z\mathfrak{H}_0) | \mathbf{q}' \rangle$$

$n \geqslant 1$:

$$\mathfrak{N}_n{}^*(E) \equiv \frac{1}{2\pi i} \frac{\partial^n}{\partial E^n} \mathcal{P} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{\exp(zE)}{z} F_n{}^*(z), \qquad (1.3.14a)$$

provided that

$$\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{\exp(zE)}{z} \int_{[\Omega]} d\mathbf{q}' \langle \mathbf{q}' | \exp(-z\mathfrak{H}_0) | \mathbf{q}' \rangle$$

and

$$\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{\exp(zE)}{z} F_n{}^*(z)$$

have continuous derivatives of all orders in the interval (1.3.12).

Arguments and assumptions of similar type lead to the following conclusion:

$$\int_{-\infty}^{\infty} dE \mathfrak{N}(E) \int_{-\infty}^{E} dE' g(E') \cong -\sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dE g(E) \int_{-\infty}^{E} dE' \mathfrak{N}_n{}^*(E'). \qquad (1.3.14b)$$

From (1.1.9), (1.3.14a), and (1.3.14b), we obtain the following:

Rule for large systems.—$N(E)$ may be replaced by

$$N^*(E) \equiv \sum_{n=0}^{\infty} N_n{}^*(E), \qquad (1.3.15)$$

where

$$N_n{}^*(E) \equiv \sum_{|m| \leqslant j} \mathfrak{N}_n{}^*(E + g\hbar\omega m)$$

and $\mathfrak{N}_n{}^*(E)$ is given by (1.3.14) in integrals of the type

$$\int_{-\infty}^{\infty} dE g(E) N(E), \qquad \int_{-\infty}^{\infty} dE N(E) \int_{-\infty}^{E} dE' g(E'), \qquad (1.3.16)$$

where $g(E)$ has the properties assumed in this section.

Since the study of the magnetic properties of metals depends on the computation of integrals of type (1.3.11), as shown in Sec. 1.4, we hope that this rule will be useful in studying such properties.

The fact that $\mathfrak{N}_n{}^*(E)$ contains $\mathfrak{H}_1$ exactly n times and the fact that the E-integrations contribute only in the narrow band (1.3.12) lead us to believe that (1.3.14a) and (1.3.14b) will fail, for example, in the case when $\mathfrak{H}_1$ depends solely on coordinates and its eigenvalues $H(\mathbf{q}')$ in the $\mathbf{q}'$-representation are much larger than E_0, i.e., ζ in our case. We must clearly demand that $E_0 \gg |H_1(\mathbf{q}')|$.

For the sake of completeness, we remark that it is also possible to approximate $\mathfrak{N}(E)$ by a series based entirely on Method II, involving the operator $\mathfrak{T}'(sz)$ of (1.2.19). This series should be useful under the same circumstances which we mentioned in connection with this method. However, since we shall not require it in this study, we shall not write it down explicitly.

1.4. General Formulation of the Magnetic Properties of an Electron Gas

The one-electron orbital Hamiltonian for our model of an electron gas in a metal is the customary one used in the theory of metals:

$$\mathfrak{H}(\mathfrak{p},\mathfrak{q}) = \frac{1}{2m_0}\left(\mathfrak{p} + \frac{e}{c}\mathfrak{A}\right)^2 + \mathfrak{B}(\mathfrak{q}) + \mathfrak{W}(\mathfrak{q}), \qquad (1.4.1)$$

where $\mathfrak{p}$ and $\mathfrak{q}$ are momentum and position operators of a particle, e and m_0 are its charge and mass; $\mathfrak{B}$ is the triply periodic crystal potential in which the conduction electrons move; $\mathfrak{W}$ is the wall potential, discussed in detail in Sec. 1.3; $\mathfrak{A}$ is the vector potential corresponding to a uniform external magnetic field acting on the particle; and c is the speed of light. We shall only assume that we are dealing with a Bravais lattice. The explicit form of $\mathfrak{B}(\mathfrak{q})$ need not be stated here, since we shall not require it in the present general formulation.

From (1.3.9), we proceed to prove the following fundamental result about $\mathfrak{N}(E)$ for orbital Hamiltonians of type (1.4.1):

$$\mathfrak{N}(E) = n\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{\exp(zE)}{z} \int_{[\omega]} d\mathbf{q}' \cdot \left\langle \mathbf{q}' \left| \exp\left\{ -z\left[\frac{1}{2m_0}\left(\mathfrak{p} + \frac{e}{c}\mathfrak{A}\right)^2 + \mathfrak{B}(\mathfrak{q})\right]\right\} \right| \mathbf{q}' \right\rangle, \qquad (1.4.2)$$

where $[\omega]$ is the volume of a unit cell, n is the number of unit cells in Ω, so that

$$n=\Omega/\omega, \tag{1.4.2$'$}$$

and the $\mathbf{q}'$-integration extends over an arbitrary unit cell in Ω.

For proof of (1.4.2), we begin by showing that the periodicity of $\mathfrak{B}(\mathfrak{q})$ implies

$$\left\langle \mathbf{q}'\middle|\exp\left\{-z\left[\frac{1}{2m_0}\left(\mathfrak{p}+\frac{e}{c}\mathfrak{A}\right)^2+\mathfrak{B}(\mathfrak{q})\right]\right\}\middle|\mathbf{q}'\right\rangle =\left\langle \mathbf{q}'+\mathbf{l}\middle|\exp\left\{-z\left[\frac{1}{2m_0}\left(\mathfrak{p}+\frac{e}{c}\mathfrak{A}\right)^2+\mathfrak{B}(\mathfrak{q})\right]\right\}\middle|\mathbf{q}'+\mathbf{l}\right\rangle, \tag{1.4.3}$$

where $\mathbf{l}$ is an arbitrary lattice vector.

To prove (1.4.3), we write, as in (1.1.15a),

$$\left\langle \mathbf{q}'\middle|\exp\left\{-z\left[\frac{1}{2m_0}\left(\mathfrak{p}+\frac{e}{c}\mathfrak{A}\right)^2+\mathfrak{B}(\mathfrak{q})\right]\right\}\middle|\mathbf{q}''\right) =(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\,\exp(-i\mathbf{k}\cdot\mathbf{q}') \times\exp\left\{-z\left[\frac{1}{2m_0}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''}+\frac{e}{c}\mathbf{A}(\mathbf{q}'')\right)^2+\mathbf{V}(\mathbf{q}'')\right]\right\}\exp(i\mathbf{k}\cdot\mathbf{q}'') \tag{1.4.4}$$

and we choose the symmetrical gauge

$$\mathbf{A}(\mathbf{q}'')=\tfrac{1}{2}[\mathbf{q}''\times\mathbf{H}] \tag{1.4.5}$$

to describe our uniform magnetic field $\mathbf{H}$.

The assumption that $V(\mathbf{q}'+\mathbf{l})=\mathbf{V}(\mathbf{q}')$ coupled with (1.4.5) leads to the operational identity

$$\exp\left\{-z\left[\frac{1}{2m_0}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''+\mathbf{l}}+\mathbf{A}(\mathbf{q}''+\mathbf{l})\right)^2+V(\mathbf{q}''+\mathbf{l})\right]\right\} =\exp\left[-\frac{ie}{\hbar c}\mathbf{q}''\cdot(\mathbf{l}\times\mathbf{H})\right] \times\exp\left\{-z\left[\frac{1}{2m_0}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''}+\frac{e}{c}\mathbf{A}(\mathbf{q}'')\right)^2+V(\mathbf{q}'')\right]\right\} \cdot\exp\left[\frac{ie}{\hbar c}\mathbf{q}''\cdot(\mathbf{l}\times\mathbf{H})\right]. \tag{1.4.6}$$

From (1.4.4) and (1.4.5), we get

$$\left\langle \mathbf{q}''+\mathbf{l}\middle|\exp\left\{-z\left[\frac{1}{2m_0}\left(\mathfrak{p}+\frac{e}{c}\mathfrak{A}\right)^2+\mathfrak{B}\right]\right\}\middle|\mathbf{q}''+\mathbf{l}\right\rangle =(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\,\exp\left\{-i\left[\mathbf{k}+\frac{e}{\hbar c}(\mathbf{l}\times\mathbf{H})\right]\cdot\mathbf{q}''\right\} \times\exp\left\{-z\left[\frac{1}{2m_0}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}''}+\frac{e}{c}\mathbf{A}(\mathbf{q}'')\right)^2+V(\mathbf{q}'')\right]\right\} \times\exp\left\{i\left[\mathbf{k}+\frac{e}{c}(\mathbf{l}\times\mathbf{H})\right]\cdot\mathbf{q}''\right\}. \tag{1.4.7}$$

Changing the variable of integration in (1.4.7), and using (1.4.4) we obtain the desired result (1.4.3).

Combining (1.4.3) with (1.3.3), where we place $f(\mathbf{q}')=1$ and $n=1$, and employing (1.1.9) and (1.1.13)$'$, we arrive at (1.4.2). *Q.E.D.*

Let us now formulate the equations for calculating the magnetic moment of the conduction electrons in Ω.

The basic definition of the magnetic moment, M, of a system of N electrons, whose total Hamiltonian is a sum of N one-particle Hamiltonians whose orbital and spin parts are given by (1.1.6), (1.1.7), and (1.4.7), for a given direction of $\mathbf{H}$, was proposed long ago by Pauli in his famous paper on paramagnetism in monatomic gases.[21] The definition is a direct generalization of the classical one and reads as follows:

$$M=\sum_p\left(-\frac{\partial E_p}{\partial H}\right)_{N,T,\Omega}f_0(E_p|\beta,\zeta), \tag{1.4.8}$$

where $H\equiv|\mathbf{H}|$ and where the direction of $\mathbf{H}$ is held constant; E_p is given by (1.1.7), with $j=1/2$, $g=2$; β has the usual meaning of $1/kT$;

$$f_0(E|\beta,\zeta)\equiv\frac{1}{\exp[\beta(E-\zeta)]+1}; \tag{1.4.8$'$}$$

and the sum in (1.4.8) involves *all* orbital and spin states. The thermodynamic potential ζ is determined by the familiar equation

$$N=\sum_p f_0(E_p|\beta,\zeta) \tag{1.4.9}$$

where N is the number of particles in the box Ω.

An equivalent definition of M can be obtained from that given in the foregoing. It is the well-known thermodynamic relation

$$M=-\left(\frac{\partial F}{\partial H}\right)_{N,T,\Omega}, \tag{1.4.10}$$

where the Helmholtz free energy for an electron gas is

[21] W. Pauli, Z. Physik 47, 81 (1927).

given by

$$F=N\zeta-\frac{1}{\beta}\sum_p \log\{1+\exp[\beta(\zeta-E_p)]\}. \quad (1.4.11)$$

When we combine (1.4.8) and (1.4.10), we get the useful result

$$M=-\frac{\delta}{\delta H}(F-N\zeta)$$
$$=\frac{1}{\beta}\frac{\delta}{\delta H}\sum_p \log\{1+\exp[\beta(\zeta-E_p)]\}, \quad (1.4.12)$$

where $\delta/\delta H$ represents a partial derivative which operates solely on those terms (coming from the E_p) which contain the magnetic field strength H explicitly; the implicit H-dependent terms in ζ are to be ignored

Since the sums in (1.4.9) and (1.4.11) are of the form (1.1.1), we can write them as follows: using (1.1.5) and (1.1.9), with $j=1/2$, $g=2$,

$$F-N\zeta=\frac{1}{\beta}\sum_{m=\pm\frac{1}{2}}\int_{-\infty}^{\infty}dE\frac{\partial}{\partial E}$$
$$\times\log\{1+\exp[\beta(\zeta-E)]\}\mathfrak{N}(E+2\hbar\omega m)$$
$$=-\sum_{m=\pm\frac{1}{2}}\int_{-\infty}^{\infty}dEf_0(E|\beta,\zeta)\mathfrak{N}(E+2\hbar\omega m),$$
$$N=-\sum_{m=\pm\frac{1}{2}}\int_{-\infty}^{\infty}dE\frac{\partial f_0(E|\beta,\zeta)}{\partial E}$$
$$\times\mathfrak{N}(E+2\hbar\omega m). \quad (1.4.13)$$

By making a partial integration, we can transform the last equation for $F-N\zeta$ to read

$$F-N\zeta=\sum_{m=\pm\frac{1}{2}}\int_{-\infty}^{\infty}dE\frac{\partial f_0(E|\beta,\zeta)}{\partial E}$$
$$\times\int_{-\infty}^{E+2\hbar\omega m}dE'\mathfrak{N}(E'). \quad (1.4.14)$$

Since Eqs. (1.4.13) and (1.4.14) involve the function $(\partial/\partial E)f_0(E|\beta,\zeta)$, which has a delta-like behavior for a degenerate Fermi gas, they are quite convenient to use in this case.

Combining (1.4.12) and (1.4.14), we get

$$M=\frac{1}{\beta}\frac{\delta}{\delta H}\sum_{m=\pm\frac{1}{2}}\int_{-\infty}^{\infty}dE\frac{\partial}{\partial E}f_0(E|\beta,\zeta)$$
$$\times\int_{-\infty}^{E+2\hbar\omega m}dE'\mathfrak{N}(E'). \quad (1.4.15)$$

Equations (1.4.13) and (1.4.15) constitute the basic foundation for studying the magnetic properties of electrons in metals. These equations reveal that the heart of the problem is the calculation of $\mathfrak{N}(E)$. In real metals, it is out of the question to compute this function in closed form, so that one must resort to perturbation methods.

We conclude this section by remarking that the form of Eqs. (1.4.13), (1.4.14), and (1.4.15), coupled with Eq. (1.4.2) allows us to conclude:

$F-N\zeta$, N, and M are proportional to Ω for those systems having wall potentials $W(\mathbf{q}')$ with the properties assumed in Sec. 1.3.

We are thus led to results in agreement with thermodynamic requirements for systems in equilibrium.

PART 2: APPLICATIONS

2.1. Simple Band Theory

In this section we shall consider the problem of finding the function $\mathfrak{N}^*(E)$ of Sec. 1.3 for conduction electrons moving in a periodic potential with no magnetic field present. We shall suppose that this potential is so weak that it constitutes a perturbation on the free-electron states, so that we may reasonably apply Eq. (1.3.15) to the problem with neglect of terms having $n>2$ in this equation.

To this approximation, our final answer for $\mathfrak{N}^*(E)$ agrees with that which one would obtain by the perturbation-theoretic procedures used in the familiar treatments of band theory for the case of weak binding.[22] This result was to be expected in view of the work in the Appendix.

If $H=0$, Eq. (1.4.7) reduces to

$$\mathfrak{H}(\mathfrak{p},\mathfrak{q})=\frac{1}{2m_0}\mathfrak{p}^2+\mathfrak{V}(\mathfrak{q})+\mathfrak{W}(\mathfrak{q}), \quad (2.1.1)$$

where

$$\mathfrak{p}=|\mathfrak{p}|.$$

We place

$$\mathfrak{K}\equiv\frac{1}{2m_0}\mathfrak{p}^2,\qquad \mathfrak{H}_1\equiv\mathfrak{V}(\mathfrak{q}). \quad (2.1.2)$$

We now proceed to calculate $\mathfrak{N}_0^*(E)$, $\mathfrak{N}_1^*(E)$, $\mathfrak{N}_2^*(E)$. From (1.3.13) and (2.1.2) we have

$$\mathfrak{N}_0^*(E)=\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}$$
$$\times\int_{[\Omega]}d\mathbf{q}'\left\langle\mathbf{q}'\left|\exp\left(-\frac{z}{2m_0}\mathfrak{p}^2\right)\right|\mathbf{q}'\right\rangle. \quad (2.1.3)$$

Using (1.1.15a), where we place

$$\mathfrak{H}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}'},\mathbf{q}'\right)=-\frac{\hbar^2}{2m_0}\nabla_{\mathbf{q}'}{}^2,$$

[22] See any book on the theory of metals, for example, A. H. Wilson, *The Theory of Metals* (Cambridge University Press, Cambridge, 1953), second edition, Chap. 2, Sec. 2.5.

we find that

$$\left\langle \mathbf{q}'\left|\exp\left(-\frac{z}{2m_0}\mathfrak{p}^2\right)\right|\mathbf{q}'\right\rangle$$

$$=(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}')$$

$$\times\exp\left(\frac{\hbar^2}{2m_0}z\nabla_{q'}{}^2\right)\exp(i\mathbf{k}\cdot\mathbf{q}')$$

$$=(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp\left(-\frac{\hbar^2 z\mathbf{k}^2}{2m_0}\right)=\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}z^{-\frac{3}{2}},\quad(2.1.4)$$

where $k\equiv|\mathbf{k}|$.

From (2.1.4), we see that we can forget about $\mathcal{P}$ in (2.1.3) since the z-integral converges for $\gamma>0$, an inequality which we suppose to be satisfied without exception in this paper. Combining this remark with the formula

$$\frac{1}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}dze^{zE}z^{-(n+\frac{1}{2})}=\frac{2^nE^{n-\frac{1}{2}}U(E)}{1\cdot3\cdot5\cdots(2n-1)\pi^{\frac{1}{2}}},$$

$$n=1,2,\cdots,\quad(2.1.5)$$

where $U(x)$ has been defined in (1.1.3), and using (2.1.3) and (2.1.4), we obtain

$$\mathfrak{N}_0^*(E)=\frac{4}{3\pi^{\frac{1}{2}}}\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\Omega E^{\frac{3}{2}}U(E).\quad(2.1.6\text{a})$$

The usual smoothed-out orbital density of states for free electrons is merely

$$\frac{d}{dE}\mathfrak{N}_0^*(E)=\frac{2}{\pi^{\frac{1}{2}}}\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\Omega E^{\frac{1}{2}}U(E).\quad(2.1.6)'$$

Since $\mathbf{H}\equiv\mathbf{0}$, the total density of states including spin is obtained by multiplying this answer by a factor two. We notice that the factor Ω in (2.1.6) and (2.1.6)′ is a consequence of the sharp rise of $W(\mathbf{q}')$ at the boundaries of the box, as expressed by (1.3.3).

In order to proceed, we expand $V(\mathbf{q}')$ in a Fourier series for $\mathbf{q}'$ in Ω, thus

$$V(\mathbf{q}')=\sum_{\boldsymbol{\kappa}}v(\boldsymbol{\kappa})\exp(i\boldsymbol{\kappa}\cdot\mathbf{q}'),$$

$$v(\boldsymbol{\kappa})=\frac{1}{\Omega}\int_{[\Omega]}d\mathbf{q}'\exp(-i\boldsymbol{\kappa}\cdot\mathbf{q}')V(\mathbf{q}').\quad(2.1.7)$$

If we adjust the zero of potential energy so that the average of $V(\mathbf{q}')$ over the crystal vanishes, i.e., if

$$\int_{[\Omega]}d\mathbf{q}'V(\mathbf{q}')=0,\quad(2.1.8)$$

we have[23]

$$\mathfrak{N}_1^*(E)=0.\quad(2.1.6\text{b})$$

To prove (2.1.6b), we employ Eqs. (1.3.10), (1.3.13), (2.1.2), (2.1.4), and (2.1.8), thus obtaining

$$\mathfrak{N}_1^*(E)=-\frac{1}{2\pi i}\frac{\partial}{\partial E}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}$$

$$\times\int_{[\Omega]}d\mathbf{q}'V(\mathbf{q}')\langle\mathbf{q}'|\exp(-z\mathfrak{p}^2/2m_0)|\mathbf{q}'\rangle,$$

since $\langle\mathbf{q}'|\exp(-z\mathfrak{q}^2/2m_0)|\mathbf{q}'\rangle$ is independent of $\mathbf{q}'$ by (2.1.4).

We now turn to $\mathfrak{N}_2^*(E)$. Equations (1.3.10), (1.1.13), and (2.1.2) imply

$$\mathfrak{N}_2^*(E)=\frac{1}{2}\frac{\partial^2}{\partial E^2}\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}\int_0^1 ds\int_{[\Omega]}d\mathbf{q}'\int_{[\Omega]}d\mathbf{q}''$$

$$\times\sum_{\boldsymbol{\kappa}}\sum_{\boldsymbol{\kappa}'}v(\boldsymbol{\kappa})v(\boldsymbol{\kappa}')\exp(i\boldsymbol{\kappa}\cdot\mathbf{q}')$$

$$\times\exp(i\boldsymbol{\kappa}'\cdot\mathbf{q}'')(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp[-i\mathbf{k}\cdot(\mathbf{q}'-\mathbf{q}'')]$$

$$\times\exp[-(1-s)z(\hbar^2\mathbf{k}^2/2m_0)](2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}'$$

$$\times\exp[i\mathbf{k}'\cdot(\mathbf{q}'-\mathbf{q}'')]\exp[-sz(\hbar^2\mathbf{k}'^2/2m_0)].$$

Since the $\mathbf{q}'$, $\mathbf{q}''$ integrations are over a finite volume Ω, it is convenient to use the following familiar asymptotic result:

$$\langle\mathbf{q}'|\exp[-(1-s)(z\mathfrak{p}^2/2m_0)]|\mathbf{q}''\rangle$$

$$=(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp[-i\mathbf{k}\cdot(\mathbf{q}'-\mathbf{q}'')]$$

$$\times\exp[-(1-s)z(\hbar^2\mathbf{k}^2/2m_0)]$$

$$\sim\frac{1}{\Omega}\sum_{\mathbf{k}}\exp[-i\mathbf{k}\cdot(\mathbf{q}'-\mathbf{q}'')]$$

$$\times\exp[-(1-s)(z\hbar^2k^2/2m_0)],\quad(2.1.11)$$

where the vectors $\mathbf{k}$ of this sum range over the usual Born-von Kármán spectrum appropriate to a cubical

[23] The fact that the first-order correction to the Schwinger trace formula (1.2.9) vanishes under the above conditions has been noticed by several authors. See, for example, references 5 and 17. In reference 17 it is pointed out that this is not true when we deal, for example, with Hamiltonians with binary interactions, if we use Fermi or Bose statistics.

box of volume Ω. Then,

$$\mathfrak{N}_2^*(E)=\frac{1}{2}\frac{\partial^2}{\partial E^2}\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}$$

$$\cdot\int_0^1 ds\sum_{\boldsymbol{\kappa}}\sum(\boldsymbol{\kappa}')v(\boldsymbol{\kappa})v(\boldsymbol{\kappa}')$$

$$\cdot\frac{1}{\Omega}\sum_{\mathbf{k}}\exp[-(1-s)z(\hbar^2\mathbf{k}^2/2m_0)]$$

$$\cdot\frac{1}{\Omega}\sum_{\mathbf{k}'}\exp[-sz(\hbar^2\mathbf{k}'^2/2m_0)]$$

$$\cdot\int_{[\Omega]}d\mathbf{q}'\exp[i(\boldsymbol{\kappa}-\mathbf{k}+\mathbf{k}')\cdot\mathbf{q}']$$

$$\cdot\int_{[\Omega]}d\mathbf{q}''\exp[i(\boldsymbol{\kappa}'+\mathbf{k}-\mathbf{k}')\cdot\mathbf{q}''].$$

Using the basic orthogonality relation

$$\frac{1}{\Omega}\int_{[\Omega]}d\mathbf{q}'\exp(i\boldsymbol{\kappa}\cdot\mathbf{q}')=\delta(\boldsymbol{\kappa},\mathbf{o}),\qquad(2.1.12)$$

we are led to

$$\mathfrak{N}_2^*(E)=\frac{1}{2}\frac{\partial^2}{\partial E^2}\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}$$

$$\cdot\int_0^1 ds\sum_{\boldsymbol{\kappa}}v(\kappa)v(-\kappa)\sum_{\mathbf{k}}\exp[-(1-s)z(\hbar^2\mathbf{k}^2/2m_0)]$$

$$\times\exp[-sz\hbar^2(|\mathbf{k}-\boldsymbol{\kappa}|^2/2m_0)].$$

If we replace the sum over $\mathbf{k}$ by an integral

$$(2\pi)^{-3}\Omega\int_{-\infty}^{\infty}d\mathbf{k},$$

and use the reality condition

$$v(-\kappa)=v(\kappa)^*$$

and the fact that

$$v(\mathbf{o})=0,$$

as follows from (2.1.7) and (2.1.8), we find

$$\mathfrak{N}_2^*(E)=\tfrac{1}{2}\Omega(2\pi)^{-3}\sum_{\boldsymbol{\kappa}\neq\mathbf{o}}|v(\boldsymbol{\kappa})|^2\frac{\partial^2}{\partial E^2}$$

$$\times\int_0^1 ds\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}\int_{-\infty}^{\infty}d\mathbf{k},$$

$$\times\exp[-(\hbar^2z/2m_0)][(1-s)k^2+s|\mathbf{k}-\boldsymbol{\kappa}|^2].\qquad(2.1.13)$$

We carry out the integrations in (2.1.13) in the following order: (i) over z; (ii) over $\mathbf{k}$; (iii) over s. Carrying out (i) and (ii), we have

$$\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}\int_{-\infty}^{\infty}d\mathbf{k}$$

$$\times\exp\{-(\hbar^2z/2m_0)[(1-s)\mathbf{k}^2+s|\mathbf{k}-\boldsymbol{\kappa}|^2]\}$$

$$=\int_{-\infty}^{\infty}d\mathbf{k}'U\left(E-\frac{\hbar^2}{2m_0}s(1-s)\kappa^2-\frac{\hbar^2}{2m_0}k'^2\right)$$

$$=\frac{4\pi}{3}\left[\frac{2m_0E}{\hbar^2}-s(1-s)\kappa^2\right]^{\frac{3}{2}}U\left(E-\frac{\hbar^2}{2m_0}s(1-s)\kappa^2\right),\qquad(2.1.14)$$

where we have placed $\mathbf{k}'\equiv\mathbf{k}-\boldsymbol{\kappa}$ and $\kappa\equiv|\boldsymbol{\kappa}|$.

Combining (2.1.13) and (2.1.14), we find

$$\mathfrak{N}_2^*(E)=\frac{2m_0}{\hbar^2}\pi\Omega(2\pi)^{-3}\sum_{\boldsymbol{\kappa}\neq\mathbf{o}}|v(\boldsymbol{\kappa})|^2$$

$$\cdot\frac{\partial}{\partial E}\int_0^1 ds[\kappa_0^2-s(1-s)\kappa^2]^{\frac{1}{2}}U(\kappa_0^2-s(1-s)\kappa^2),\qquad(2.1.15)$$

where $\kappa_0^2\equiv 2m_0|E|/\hbar^2$.

In carrying out (iii) we must consider carefully the cases $\kappa<2\kappa_0$, $\kappa\geqslant 2\kappa_0$. We then arrive at the elementary formula

$$\int_0^1 ds[\kappa_0^2-s(1-s)\kappa^2]^{\frac{1}{2}}U(\kappa_0^2-s(1-s)\kappa^2)$$

$$=\frac{\kappa}{2}\left[\frac{\kappa_0}{\kappa}-\left(\frac{1}{4}-\frac{\kappa_0^2}{\kappa^2}\right)\log\frac{2\kappa_0+\kappa}{|2\kappa_0-\kappa|}\right],$$

which, in conjunction with (2.1.15), yields

$$\mathfrak{N}_2^*(E)=\frac{m_0^2\Omega}{4\pi^2\hbar^4}\sum_{\boldsymbol{\kappa}\neq\mathbf{o}}\frac{|v(\boldsymbol{\kappa})|^2}{\kappa}\log\frac{2\kappa_0+\kappa}{|2\kappa_0-\kappa|}.\qquad(2.1.16)$$

The inclusion of spin leads to no complications. In fact, from (1.3.34), putting $g=2$, $j=\frac{1}{2}$, $\omega=0$, we see that the total number of states with energy less than E is

$$N^*(E)=2\mathfrak{N}^*(E)\cong 2\mathfrak{N}_0^*(E)+2\mathfrak{N}_2^*(E),\qquad(2.1.17)$$

to the degree of approximation contemplated here.

2.2. Magnetic Properties of an Ideal Electron Gas

The properties of free electrons in magnetic fields have been of interest in physics since the period where Bohr[24] discovered a special case of a celebrated theorem[25] due to van Leeuwen. As is well known, this

[24] N. Bohr, Dissertation, Copenhagen, 1911.

[25] J. H. van Leeuwen, Dissertation, Leiden, 1919.

theorem states that a system of charges subject to the laws of classical dynamics and statistical mechanics, and in a state of thermodynamic equilibrium, has zero magnetic moment. In proving this theorem, the fact that *all* momenta are allowed in classical statistics plays a decisive role.

This paradoxical picture prevailed until 1930, when Landau[26] proved that an electron gas in equilibrium in a container exhibits a diamagnetic behavior, if one employs a correct quantum-mechanical and quantum-statistical approach. This is a purely quantum-theoretical result which is connected with the quantization of the "orbits." In Landau's work, explicit account was taken of the walls by a certain spatial cut-off procedure.

Peierls[1] arrived at the same conclusions as Landau in an entirely different way using the operator method mentioned in the Introduction. He also treated the case of strongly bound electrons.[27]

In 1930 de Haas and van Alphen[28] discovered that the magnetic susceptibility of Bi at low temperatures had an oscillating component with period proportional to $1/H$. The de Haas-van Alphen effect has since been observed in other metals.[29] The work of Landau and Peierls only gave the so-called "normal" susceptibility, due to the approximations which they used. Peierls[30] was the first to show that the de Haas-van Alphen effect could be understood by a more refined approach. The whole theory has been further perfected by Blackman,[31] Landau,[32] Akhieser,[33] Rumer,[34] Sondheimer and Wilson,[2] and Dingle.[8,35]

With the exceptions of Peierls and Sondheimer and Wilson, these investigators employed the Landau cut-off procedure mentioned previously. The studies of Osborne and Steele,[3] Dingle,[36] and Ham[37] have dealt with the validity of such procedures for treating the walls. It appears that they are allowable for system such that

$$\frac{eHR}{c} \gg m_0 v_{\text{Fermi}}, \qquad (2.2.1)$$

where v_{Fermi} is the velocity of the electrons at the Fermi energy, R is the radius of the container, and the remaining symbols have been defined in Sec. (1.4).

We believe that the wall-potential method in Sec. (1.3) and (1.4) is equivalent to the foregoing cut-off procedure, because our final answers agree with those in the references cited previously for the case of perfectly free electrons.

In this section, we shall adopt the one-electron orbital Hamiltonian in (1.4.1) with $\mathfrak{V}(\mathfrak{q})\equiv 0$, we shall take the direction of $\mathbf{H}$ along with q_3'-axis, and we shall use the symmetrical gauge (1.4.5). We then have

$$\mathcal{H}\left(\frac{\hbar}{i}\nabla_{\mathbf{q}'},\mathbf{q}'\right)=-\frac{\hbar^2}{2m_0}\nabla_{\mathbf{q}'}{}^2+\tfrac{1}{2}m_0\omega^2[q_1'^2+q_2'^2]+\omega L_3+W(\mathbf{q}'), \qquad (2.2.2)$$

where

$$L_3\equiv\frac{\hbar}{i}\left[q_1'\frac{\partial}{\partial q_2'}-q_2'\frac{\partial}{\partial q_1'}\right].$$

We shall take (2.2.1) as our criterion for "large" systems, so that we shall suppose, in particular, that (1.3.9) holds when (2.2.1) does. Since we shall only deal with systems for which this is the case, we need not mention it explicitly in what follows.

Employing (1.1.15b), (2.2.2), and (1.3.9), one can write for the orbital number of states with energy less than E

$$\begin{aligned}\mathfrak{N}(E)\cong&\int_{[\Omega]}d\mathbf{q}'\frac{1}{2\pi i}\mathcal{P}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z}\\ &\cdot(2\pi)^{-3}\int_{-\infty}^{\infty}d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}')\\ &\times\exp\left\{-z\left[-\frac{\hbar^2}{2m_0}\nabla_{\mathbf{q}'}{}^2+\omega L_3+\tfrac{1}{2}m_0\omega^2(q_1'^2+q_2'^2)\right]\right\}\\ &\times\exp(i\mathbf{k}\cdot\mathbf{q}'). \end{aligned}\qquad (2.2.3)$$

It is clear that the Hamiltonian in (2.2.2) is invariant under rotations about the q_3'-axis, so that L_3 commutes with H. This leads to a happy simplification of the exponential operators, i.e.,

$$\begin{aligned}&\exp\left\{-z\left[-\frac{\hbar^2}{2m_0}\nabla_{\mathbf{q}'}{}^2+\tfrac{1}{2}m_0\omega^2(q_1'^2+q_2'^2)+\omega L_3\right]\right\}\\ &=\exp(-z\omega L_3)\\ &\quad\times\exp\left\{-z\left[-\frac{\hbar^2}{2m_0}\nabla_{\mathbf{q}'}{}^2+\tfrac{1}{2}m_0\omega^2(q_1'^2+q_2'^2)\right]\right\}\\ &\equiv\mathfrak{G}.\end{aligned}\qquad (2.2.4)$$

It is convenient to introduce the so-called natural units as follows

$$(q_1',q_2',q_3')\equiv\frac{\hbar}{m_0\omega}(\xi_1,\xi_2,\xi_3), \qquad (2.2.5)$$

[26] L. Laudau, Z. Physik **64**, 629 (1930).
[27] See also R. H. Wilson [Proc. Cambridge Phil. Soc. **49**, 292 (1953)] for a treatment of steady susceptibility of metals by means of a density-matrix approach.
[28] W. J. de Haas and P. M. van Alphen, Proc. Acad. Sci. Amsterdam **33**, 1106 (1930).
[29] See, for example, D. Shoenberg, Phil. Trans. **A245**, 1 (1952).
[30] R. Peierls, Z. Physik **81**, 186 (1933).
[31] M. Blackman, Proc. Roy. Soc. (London) **A166**, 1 (1938).
[32] L. Landau, Appendix to D. Shoenberg, Proc. Roy. Soc. (London) **A770**, 347 (1939).
[33] A. Akhieser, C. R. Acad. Sci. U.S.S.R. **23**, 874 (1939).
[34] Y. B. Rumer, J. Exptl. Theoret. Phys. U.S.S.R. **18**, 1081 (1948).
[35] R. B. Dingle, Proc. Roy. Soc. (London) **A211**, 517 (1952).
[36] R. B. Dingle, Proc. Roy. Soc. (London) **A212**, 47 (1952); **A216**, 118 (1953); **A219**, 463 (1953).
[37] F. S. Ham, Phys. Rev. **92**, 1113 (1953).

so that

$$\pi_k \equiv -i\frac{\partial}{\partial \xi_k}, \quad k=1,2,3,$$

$$[\pi_k, \xi_l] = -i\delta_{kl}, \tag{2.2.6a}$$

and

$$\omega L_3 = \hbar\omega(\xi_1\pi_2 - \xi_2\pi_1) \equiv \hbar\omega\mathfrak{L}_3. \tag{2.2.6b}$$

Combining Eqs. (2.2.4) to (2.2.6b) we get

$$\mathfrak{G} = \exp\left(-\frac{\hbar\omega z}{2}\pi_3^2\right)\exp(-\hbar\omega z\mathfrak{L}_3) \times\exp\left[-\frac{\hbar\omega z}{2}(\pi_1^2+\xi_1^2)\right] \times\exp\left[-\frac{\hbar\omega z}{2}(\pi_2^2+\xi_2^2)\right], \tag{2.2.7}$$

where we have also employed the fact that the four operators $\mathfrak{L}_3$, π_3^2, $\pi_1^2+\xi_1^2$, $\pi_2^2+\xi_2^2$ commute in virtue of (2.2.6a).

Using (2.2.5), (2.2.7), and the change of variables $\boldsymbol{\sigma} = (\hbar/m_0\omega)^{\frac{1}{2}}\mathbf{k}$, we obtain

$$(2\pi)^{-3}\int_{-\infty}^{\infty} d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}'')\exp\left\{-z\left[-\frac{\hbar^2}{2m_0}\nabla_{q'}^2 +\omega L_3+\tfrac{1}{2}m_0\omega^2(q_1'^2+q_2'^2)\right]\right\}\exp(i\mathbf{k}\cdot\mathbf{q}')$$

$$=\left(\frac{m_0\omega}{\hbar}\right)^{\frac{3}{2}}(2\pi)^{-1}\int_{-\infty}^{\infty}d\sigma_3\exp(-i\sigma_3\xi_3'') \times\exp\left[-\frac{\hbar\omega z}{2}\left(\frac{1}{i}\frac{\partial}{\partial\xi_3'}\right)^2\right]\exp(i\sigma_3\xi_3')$$

$$\times\exp(-\hbar\omega z\mathfrak{L}_3)\left\{(2\pi)^{-1}\int_{-\infty}^{\infty}d\sigma_1\exp(-i\sigma_1\xi_1'') \times\exp\left\{-\frac{\hbar\omega z}{2}\left[\left(\frac{1}{i}\frac{\partial}{\partial\xi_1'}\right)^2+\xi_1'^2\right]\right\}\exp(i\sigma_1\xi_1')\right.$$

$$\left.\times(2\pi)^{-1}\int_{-\infty}^{\infty}d\sigma_2\exp(-i\sigma_2\xi_2'') \times\exp\left\{-\frac{\hbar\omega z}{2}\left[\left(\frac{1}{i}\frac{\partial}{\partial\xi_2'}\right)^2+\xi_2'^2\right]\right\}\exp(i\sigma_2\xi_2')\right\}. \tag{2.2.8}$$

We shall require two identities. The first is

$$\exp(i\theta\mathfrak{L}_3)F(\xi_1,\xi_2,\xi_3) = F(\xi_1^*,\xi_2^*,\xi_3^*), \tag{2.2.9}$$

where

$$\xi_1^* = \cos\theta\xi_1 - \sin\theta\xi_2,$$
$$\xi_2^* = \sin\theta\xi_1 + \cos\theta\xi_2,$$
$$\xi_3^* = \xi_3,$$

and where θ is a complex number. Equation (2.2.9) expresses the fact that $\exp(i\theta\mathfrak{L}_3)$ is a finite rotation operator corresponding to the (complex) angle θ.

The second identity is

$$\langle\xi'|\mathfrak{P}_{S\cdot H\cdot O}|\xi\rangle \equiv (2\pi)^{-1}\int_{\infty}^{\infty}d\sigma\exp(-i\sigma\xi') \times\exp\left\{-\frac{\hbar\omega z}{2}\left[\left(\frac{1}{i}\frac{\partial}{\partial\xi}\right)^2+\xi^2\right]\right\}\exp(i\sigma\xi)$$

$$=(2\pi\sinh(\hbar\omega z))^{-\frac{1}{2}} \times\exp\left\{-\frac{1}{4}\left[(\xi'+\xi)^2\tanh\left(\frac{\hbar\omega z}{2}\right) +(\xi'-\xi)^2\coth\left(\frac{\hbar\omega z}{2}\right)\right]\right\}, \tag{2.2.10}$$

which follows by transformation theory from a celebrated summation formula discovered by Mehler.[10] Equation (2.2.8) becomes

$$\left(\frac{m_0\omega}{\hbar}\right)^{\frac{3}{2}}(2\pi\hbar\omega z)^{-\frac{1}{2}}\exp(-\hbar\omega z\mathfrak{L}_3) \times\langle\xi_1'|\mathfrak{P}_{S\cdot H\cdot O}|\xi_1\rangle\langle\xi_2'|\mathfrak{P}_{S\cdot H\cdot O}|\xi_2\rangle$$

$$=\left(\frac{m_0\omega}{\hbar}\right)^{\frac{3}{2}}\cdot(2\pi\hbar\omega z)^{-\frac{1}{2}} \cdot\langle\xi_1'|\mathfrak{P}_{S\cdot H\cdot O}|\cosh(\hbar\omega z)\xi_1 - i\sinh(\hbar\omega z)\xi\rangle_2 \cdot\langle\xi_2'|\mathfrak{P}_{S\cdot H\cdot O}|i\sinh(\hbar\omega z)\xi_1+\cosh(\hbar\omega z)\xi_2\rangle.$$

Substituting (2.2.10) into this equation and taking the limits $\xi_1'\to\xi_1$; $\xi_2'\to\xi_2$ in the final results leads after some manipulations to the following:

$$(2\pi)^{-3}\int_{\infty}^{\infty}d\mathbf{k}\exp(-i\mathbf{k}\cdot\mathbf{q}')\exp\left\{-z\left[-\frac{\hbar^2}{2m_0}\nabla_{q'}^2 +\omega L_3+\tfrac{1}{2}m_0\omega^2(q_1'^2+q_2'^2)\right]\right\}\exp(i\mathbf{k}\cdot\mathbf{q}')$$

$$=\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}z^{-\frac{3}{2}}\frac{\hbar\omega z}{\sinh(\hbar\omega z)}. \tag{2.2.11}$$

This result for the coordinate diagonal matrix elements of the density operator is independent of coordinates as it must be for a "nonlocalized" particle in a box.

Equations (2.2.3) and (2.2.11) imply

$$\mathfrak{N}(E)\cong\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\frac{\Omega}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}\frac{dze^{zE}}{z^{5/2}}\frac{\hbar\omega z}{\sinh(\hbar\omega z)},\qquad(2.2.12)$$

where we no longer require the principal value sign.

As mentioned in Sec. 1.1, once $\mathfrak{N}(E)$ is known for separable systems of the type considered in this paper, the question of determining their equilibrium properties is virtually solved.

We now proceed to compute the magnetic moment of our electron gas. We shall omit the straightforward but lengthy contour integrations since they are available in reference 2. We wish to emphasize the circumstance that our method of computing the expression for the number of orbital states having energy less than E in (2.2.12) is completely different from the one in this reference.

From (2.1.12) performing the indicated contour integrals, we find

$$\int_{-\infty}^{E}dE'\mathfrak{N}(E')\cong\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\cdot\frac{\Omega}{2\pi i}\int_{\gamma-i\infty}^{\gamma+i\infty}dz\frac{e^{zE}}{z^{7/2}}\frac{\hbar\omega z}{\sinh(\hbar\omega z)}$$

$$=\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\Omega(\mu H)^{5/2}\Bigg[-\frac{\pi^{-\frac{1}{2}}}{3}\left(\frac{E}{\mu H}\right)^{\frac{1}{2}}$$

$$+\frac{8}{15}\pi^{-\frac{1}{2}}\left(\frac{E}{\mu H}\right)^{5/2}+\frac{1}{\pi}\int_0^\infty dy$$

$$\times\exp\left(-\frac{E}{\mu H}y\right)y^{-5/2}\left\{\frac{1}{y}-\frac{y}{6}-\frac{1}{\sinh y}\right\}$$

$$-2\sum_{m=1}^{\infty}\frac{(-)^m}{(n\pi)^{5/2}}\cos\pi\left\{\frac{nE}{\mu H}-\frac{1}{4}\right\}\Bigg]U(E),\qquad(2.2.13)$$

where $\mu\equiv e\hbar/2m_0c$.

We shall now require the asymptotic formula

$$\int_a^\infty dE\exp\left[\frac{2\pi l}{\mu H}(E-\zeta)\right]\frac{\partial}{\partial E}f_0(E|\beta,\zeta)$$

$$\cong-\frac{\pi^2 l}{\beta\mu H}\frac{1}{\sinh\left[\frac{\pi^2 l}{\beta\mu H}\right]},\qquad(2.2.14)$$

valid when $|a|\ll\zeta$ and $\beta\zeta\gg1$. We shall identify a with $\pm\mu H$ in the following, so that both inequalities will hold for degenerate electron gases subjected to the magnetic fields currently available.

Combining Eqs. (1.4.13), (1.4.14), (2.2.13), and (2.2.14), we conclude the following:

$$N\cong-\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\Omega(\mu H)^{5/2}\Bigg\{\int_{-\infty}^{\infty}dE\Bigg[-\frac{\pi^{-\frac{1}{2}}}{6}\frac{\{E-\mu H\}^{-\frac{1}{2}}}{(\mu H)^{\frac{1}{2}}}$$

$$-\frac{\pi^{-\frac{1}{2}}}{6}\frac{\{E+\mu H\}^{-\frac{1}{2}}}{(\mu H)^{\frac{1}{2}}}+\frac{4}{3}\pi^{-\frac{1}{2}}\frac{\{E-\mu H\}^{\frac{3}{2}}}{(\mu H)^{5/2}}$$

$$+\frac{4}{3}\pi^{-\frac{1}{2}}\frac{\{E+\mu H\}^{\frac{3}{2}}}{(\mu H)^{5/2}}-\frac{2\cosh 1}{\pi(\mu H)}\int_0^\infty dy\frac{\exp\left(-\frac{E}{\mu H}y\right)}{y^{5/2}}$$

$$\times\left(\frac{1}{y}-\frac{1}{6}y-\frac{1}{\sinh y}\right)\Bigg]\frac{\partial f_0(E|\beta,\zeta)}{\partial E}$$

$$-\frac{4\pi^{\frac{1}{2}}}{\beta\mu H}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{1}{2}}}\frac{\sin\pi\left(\frac{n\zeta}{\mu H}-\frac{1}{4}\right)}{\sinh\left[\frac{\pi^2 n}{\beta\mu H}\right]}\Bigg\},\qquad(2.2.15)$$

$$F-N\zeta\cong-\left(\frac{2\pi m_0}{h^2}\right)^{\frac{3}{2}}\Omega(\mu H)^{5/2}\Bigg\{\int_{-\infty}^{\infty}dE\Bigg[-\frac{\pi^{-\frac{1}{2}}}{6}\frac{\{E-\mu H\}^{\frac{1}{2}}}{(\mu H)^{\frac{1}{2}}}$$

$$-\frac{\pi^{-\frac{1}{2}}}{6}\frac{\{E+\mu H\}^{\frac{1}{2}}}{(\mu H)^{\frac{1}{2}}}+\frac{8}{30}\frac{\pi^{-\frac{1}{2}}\{E-\mu H\}^{5/2}}{(\mu H)^{5/2}}$$

$$+\frac{8}{30}\pi^{-\frac{1}{2}}\frac{\{E+\mu H\}^{5/2}}{(\mu H)^{5/2}}+\frac{2}{\pi}\cosh 1\int_0^\infty dy$$

$$\times\exp\left(-\frac{E}{\mu H}y\right)\left(\frac{1}{y}-\frac{1}{6}y-\frac{1}{\sinh y}\right)\Bigg]\frac{\partial f_0(E|\beta,\zeta)}{\partial E}$$

$$+\frac{4\pi^{-\frac{1}{2}}}{\beta\mu H}\sum_{n=1}^{\infty}\frac{1}{n^{\frac{3}{2}}}\frac{\cos\pi\left(\frac{n\zeta}{\mu H}-\frac{1}{4}\right)}{\sinh\left[\frac{n\pi^2}{\beta\mu H}\right]}\Bigg\},\qquad(2.2.16)$$

where $\{x\}\equiv0$ for $x<0$ and $\{x\}\equiv x$ for $x>0$, so that the fractional powers of $E\pm\mu H$ in (2.2.15) cause no difficulties.

The results for the magnetic moment are given below:

$$M=M_1+M_2,\qquad(2.2.17)$$

where the meaning of M_1 and M_2 is explained in the following.

M_1 represents the nonoscillatory, or "normal" portion of M. If

$$\mu H \ll \frac{1}{\beta}, \quad \frac{1}{\beta} \ll \zeta, \tag{2.2.18a}$$

it dominates M_2. If inequalities (2.2.18a) hold, then

$$M_1 \cong M_{\mathrm{Pauli}} + M_{\mathrm{Landau}},$$

$$M_{\mathrm{Landau}} \equiv -\frac{8}{3} \frac{\pi m_0^{\frac{3}{2}}}{h^2} (2\zeta_0)^{\frac{1}{2}} \mu^2, \tag{2.2.19}$$

$$M_{\mathrm{Pauli}} \equiv -3 M_{\mathrm{Landau}},$$

where ζ_0 is the Fermi energy for $T=0$ and $H=0$, M_{Landau} is the orbital diamagnetic moment discovered by Landau[26] and M_{Pauli} is the spin paramagnetic moment pointed out by Pauli.[21,38]

If

$$\pi^2/\beta\mu H \gtrsim 1, \quad \frac{1}{\beta} \ll \zeta, \tag{2.2.18b}$$

then M_2, which is given by

$$M_2 = \frac{3\pi}{\beta\mu H}\left(\frac{\zeta}{\mu H}\right)^{\frac{1}{2}} \sum_{l=1}^{\infty} \frac{\sin\left(\frac{\pi}{4} - \frac{l\pi\zeta}{\mu H}\right)}{l^{\frac{1}{2}} \sinh\left[\frac{\pi^2 l}{\beta\mu H}\right]}, \tag{2.2.20}$$

is appreciable, and may even dominate M_1. From (2.2.20), we see that M_2 exhibits characteristic oscillations whose frequency is proportional to $1/H$. These oscillations are qualitatively of the same type as those observed by de Haas and van Alphen.[28]

We shall say nothing concerning the ingenious, but rather artificial elaborations of the foregoing work using effective mass concepts,[31] although we could easily include such schemes in our calculation of $N(E)$. We hope that the perturbation-theoretic procedures in Secs. 1.2 and 1.3 will aid in approaching the problem of calculating M on the basis of the Hamiltonian in (1.4.1), without the introduction of these concepts.

APPENDIX

Let $\mathfrak{H}$, $\mathfrak{H}_0$, and $\mathfrak{H}_1$ have the same meanings as in Sec. 1.1, so that

$$\mathfrak{H} = \mathfrak{H}_0 + \mathfrak{H}_1, \tag{A.1}$$

where $\mathfrak{H}_1$ is "small" compared with $\mathfrak{H}_0$. We suppose that both $\mathfrak{H}_0$ and $\mathfrak{H}_1$ have pure-point spectra.

[38] One can derive the normal magnetic moment by expanding $\mathfrak{N}(E)$ in (2.2.12) in powers of H up to quadratic terms using (1.4.15).

Let ${}_0E_p$ denote the energy eigenvalues corresponding to the eigenket $|p\alpha\rangle$ of $\mathfrak{H}_0$, where $\alpha = 1, 2 \cdots g(p)$. As the perturbation changes from 0 to some "small" operator, the ${}_0E_p$ go to eigenvalues $E_p{}^\alpha$ of $\mathfrak{H}$.

We shall now calculate

$$\operatorname{trace} \exp(-z\mathfrak{H}) = \sum_p^\alpha \exp(-zE_p{}^\alpha) \tag{A.2}$$

for $\mathrm{Re}\{z\} > 0$ in terms of

$$\operatorname{trace} \exp(-z\mathfrak{H}_0) = \sum_p^\alpha \exp(-z_0E_p), \tag{A.3}$$

which corresponds to the unperturbed problem, and

$$\Delta E_p{}^\alpha \equiv E_p{}^\alpha - {}_0E_p. \tag{A.4}$$

From (A.4), we have

$$\exp(-zE_p{}^\alpha) = \exp(-z_0E_p)\exp(-z\Delta E_p{}^\alpha)$$
$$= \exp(-z_0E_p) \sum_{n=0}^{\infty} \frac{(-)^n}{n!} z^n (\Delta E_p{}^\alpha)^n. \tag{A.5}$$

Let $\Delta E_{p,r}{}^\alpha$ $(r = 1, 2, \cdots)$ be the contribution to $\Delta E_p{}^\alpha$ in (A.4) according to rth-order perturbation theory, so that

$$\Delta E_p{}^\alpha = \sum_{r=1}^{\infty} \Delta E_{p,r}{}^\alpha. \tag{A.6}$$

From (A.2), (A.3), (A.5), and (A.6) we obtain

$$\operatorname{trace} \exp(-z\mathfrak{H}) = \operatorname{trace} \exp(-z\mathfrak{H}_0)$$
$$-z\sum_p^\alpha \exp(-z_0E_p)\Delta E_{p,1}{}^\alpha + \sum_p^\alpha \exp(-z_0E_p)$$
$$\times \left\{ -z\Delta E_{p,2}{}^\alpha + \frac{z^2}{2}(\Delta E_{p,1}{}^\alpha)^2 \right\} + O_3, \tag{A.7}$$

where O_3 corresponds to terms containing products of $\Delta E_{p,r}{}^\alpha$ such that the sum of their r's is greater than 2. It is easy to see that these terms involve products of three or more matrix elements of $\mathfrak{H}_1$.

It is well known that if we choose a set of eigenkets $|p\alpha\rangle$ such that

$$\langle p\alpha|\mathfrak{H}_1|p\beta\rangle = \delta_{\alpha\beta}\langle p\alpha|\mathfrak{H}_1|p\alpha\rangle \tag{A.8}$$

for every *fixed* p, which we can always do by appropriate linear combinations of the $g(p)$ linearly independent eigenkets of $\mathfrak{H}_0$ belonging to ${}_0E_p$, then

$$\Delta E_{p,1}{}^\alpha = \langle p\alpha|\mathfrak{H}_1|p\alpha\rangle,$$

$$\Delta E_{p,2}{}^\alpha = -\sum_{p' \neq p}^{\beta} \frac{|\langle p\alpha|\mathfrak{H}_1|p'\beta\rangle|^2}{{}_0E_{p'} - {}_0E_p}. \tag{A.9}$$

In order to complete our derivation, we shall also require the following formulas:

$$\sum_p^\alpha \exp(-z_0E_p)\Delta E_{p,1}{}^\alpha = \text{trace}\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\}, \quad \text{(A.10a)}$$

$$z\sum_p^\alpha \exp(-z_0E_p|\langle p\alpha|\mathfrak{H}_1|p\alpha\rangle|^2 + 2\sum_{p'\neq p}^\alpha \frac{\exp(-z_0E_p)}{{}_0E_p{}' - {}_0E_p}|\langle p\alpha|\mathfrak{H}_1|p'\alpha\rangle|^2$$
$$= z\,\text{trace}\left\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\int_0^1 ds \exp(sz\mathfrak{H}_0) \cdot \mathfrak{H}_1 \exp(-sz\mathfrak{H}_0)\right\}. \quad \text{(A.10b)}$$

To prove (A.10a), we merely evaluate trace$\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\}$ in terms of the basis $|p\alpha\rangle$, using (A.8) and (A.9).

To prove (A.10b), we employ the two last equations as follows:

$$z\,\text{trace}\left\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\int_0^1 ds \exp(+sz\mathfrak{H}_0)\mathfrak{H}_1 \exp(-sz\mathfrak{H}_0)\right\}$$
$$= z\sum_{p,p'}^{\alpha,\beta} \langle p\alpha|\mathfrak{H}_1|p'\beta\rangle \exp(-z_0E_{p'})\int_0^1 ds \exp(sz_0E_{p'}) \cdot \langle p'\beta|\mathfrak{H}_1|p\alpha\rangle \exp(-sz_0E_p)$$
$$= z\sum_p^\alpha |\langle p\alpha|\mathfrak{H}_1|p\alpha\rangle|^2 \exp(-z_0E_p) + \sum_{p'\neq p}^\alpha |\langle p\alpha|\mathfrak{H}_1|p'\alpha\rangle|^2\left\{\frac{\exp(-z_0E_p)-\exp(-z_0E_{p'})}{{}_0E_{p'} - {}_0E_p}\right\},$$

which can be readily seen to be equivalent to (A.10b). *Q.E.D.*

Combining Eqs. (A.7), (A.9), and (A.10), we arrive at the following result:

$$\text{trace}\exp(-z\mathfrak{H}) = \text{trace}\exp(-z\mathfrak{H}_0) - z\,\text{trace}\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\} + \tfrac{1}{2}z^2\,\text{trace}\left\{\mathfrak{H}_1 \exp(-z\mathfrak{H}_0)\int_0^1 ds \times \exp(sz\mathfrak{H}_0)\mathfrak{H}_1 \exp(-sz\mathfrak{H}_0)\right\} + O_3. \quad \text{(A.11)}$$

Comparing (A.11) with (1.2.9), we see that the series for trace $\exp(-z\mathfrak{H})$ computed by means of degenerate perturbation theory, neglecting O_3 terms, agrees with the Schwinger trace formula, throwing away terms with $n\geqslant 3$ in the latter.

It is of interest to compare the methods of this appendix with those of Peierls.[1]