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Theory of the de Haas-van Alphen Effect for a System of Interacting Fermions*

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The de Haas-van Alphen effect for a system of interacting fermions is investigated. It is shown that, granting certain analytic properties (which were used before in establishing the existence of a Fermi surface, and which have only been established in the sense of perturbation theory), it is possible to obtain a simple expression for the oscillatory part of the thermodynamic potential. In particular, one finds that the de Haas-van Alphen oscillations have the same amplitude and period as in the usual quasi-particle picture, but that the phase is given by a more complicated proceedure.

I. INTRODUCTION

IN a recent paper[1] we have studied some properties of a system of interacting fermions, which are related to what might be called the "single-particle" aspects of such a system. These included the existence of a sharp discontinuity in the momentum distribution, defining the Fermi surface, and simple formulas for the heat capacity and spin paramagnetism in terms of certain effective single-particle excitation energies. The technique used for studying the effects of interaction among the fermions was that of Luttinger and Ward.[2] The existence of these single-particle properties is related to an analytic property of the single-particle propagators which appear in LW. This property has only been established on the assumption that one may expand certain quantities in powers of the interaction strength.[3]

In this paper we shall continue to assume this analytic property, and use it to investigate the response of an interacting many-fermion system to an external homogeneous magnetic field. As is well known,[4] the independent-particle model leads to what is known as the de Haas-van Alphen (DHVA) effect: namely, that the magnetization is not a monotonic function of the field strength H, but undergoes oscillations when viewed as a function of $1/H$. The period of the oscillations is related to a purely geometrical property of the Fermi surface (FS).[5] Similar oscillations occur in other physical properties such as the heat capacity, the magnetoresistance, the Hall coefficient, etc. For simplicity we shall refer to these collectively as DHVA oscillations. What we shall show here is the following: given the basic analytic properties of the propagator which have been established to arbitrary order in perturbation theory, the DHVA oscillations are again present in the equilibrium phenomena. More specifically, it is shown that the entire oscillatory behavior of the thermodynamic potential Ω (of the grand partition function) has exactly the same form as one would get if one assumed that the elementary excitations introduced in I behaved just like independent particles in a magnetic field. From this expression, the DHVA oscillations of the magnetization or heat capacity can be calculated by the usual formulas.

In Sec. II, the part of Ω responsible for the DHVA oscillations is isolated and expressed in terms of the true single-particle excitation energies in a magnetic field. In Sec. III the single-particle propagator is studied in detail. In particular, the gauge invariance of the original Hamiltonian is shown to determine the essential properties which we need. The true single-particle energies in

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[1] J. M. Luttinger, Phys. Rev. **119**, 1153 (1960). We shall refer to this paper as I.

[2] J. M. Luttinger and J. C. Ward, Phys. Rev. **118**, 1417 (1960). This paper will be referred to as LW. We shall use the notation of I and LW as far as is practical.

[3] J. M. Luttinger, Phys. Rev. **121**, 942 (1961).

[4] See, for example, A. H. Kahn and H. P. R. Frederikse, *Advances in Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, New York, 1959), Vol. 9, p. 257; A. B. Pippard, *Reports on Progress in Physics* (The Physical Society, London, 1960), Vol. 23, p. 176.

[5] The general treatment for an arbitrary Fermi surface is found in I. M. Lifshitz and A. M. Kosevich, Soviet Phys.—JETP **2**, 636 (1956).

an external field are then shown to be, to the accuracy required for the DHVA effect, just what one would expect for quasi-particles of charge e in the external field.

II. OSCILLATING PART OF THE THERMODYNAMIC POTENTIAL

From (I.75) the thermodynamic potential Ω is given by

$$\Omega=-\frac{1}{\beta}\sum_l \mathrm{Tr}\{\ln[\epsilon+G(\zeta_l)-\zeta_l] +S'(\zeta_l)G(\zeta_l)\}\exp(\zeta_l 0^+)+\Omega'\{G\}, \quad (1)$$

$\Omega'\{G\}=$[contribution of all closed-linked skeleton diagrams, but with $S_r(\zeta_l)\delta_{rr'}$ replaced by $S_{rr'}'(\zeta_l)$]. (2)

$S'(\zeta_l)$ is the matrix propagator and $G(\zeta_l)$ the matrix proper self-energy part, related by

$$S'(\zeta_l)=1/[\zeta_l-\epsilon-G(\zeta_l)], \quad (3)$$

where ϵ is the unperturbed single-particle Hamiltonian of the fermions. The matrix propagator formalism of I is necessary because in the presence of an external magnetic field the translational invariance of the interaction no longer insures that an incoming line in a propagator has the same quantum numbers as an outgoing one. Further we shall also be interested in the case of electrons in an external periodic potential as well as the external magnetic field and the interaction, and for this situation the matrix propagators are of course necessary.

To isolate the oscillatory part of (1) we have to consider some orders of magnitude. There are three relevant energies in our problem: the chemical potential μ, the thermal energy kT, and the magnetic energy $\omega\equiv eH/mc$. (Units such that $\hbar=1$ are chosen throughout this paper.) The range of interest for the DHVA effect is

$$kT,\ \omega\ll\mu, \quad (4)$$

and kT not exceeding ω in order of magnitude. The leading term in the DHVA effect is the one which we obtain by dropping corrections in $(kT/\mu)^2$, and powers of ω/μ beyond the first which is necessary to give an effect. The ratio kT/ω is not assumed small, however.

Let us write G as follows

$$G=G_0+G_T+G_{\mathrm{osc}}. \quad (5)$$

In (5), G_0 means the part of G which is field dependent but has no explicit DHVA oscillations in it, taken at absolute zero. G_T is the first temperature correction to this. By the usual Sommerfeld treatment of the integrals arising in Fermi-Dirac statistics, one easily sees that

$$G_T\sim(kT/\mu)^2G_0. \quad (6)$$

G_{osc} is the leading oscillatory term of G, in the sense we have been discussing. It is not difficult to see that

$$G_{\mathrm{osc}}\sim(\omega/\mu)^{\frac{1}{2}}G_0, \quad (7)$$

under the conditions given above. This is done in detail for a simple case in Appendix A, but the result is quite general, and obtained by essentially the same method. Therefore,

$$G_{\mathrm{osc}}/G_T\sim(\omega/kT)^2(\mu/\omega)^{\frac{1}{2}}\gg1, \quad (8)$$

so we may drop G_T for our purposes.

Further, by the stationary property of the expression (1) for Ω, viewed as a functional of G, we have

$$\Omega=\frac{-1}{\beta}\sum_l \mathrm{Tr}\{\ln[\epsilon+G_0(\zeta_l)-\zeta_l]+S_0'(\zeta_l)G_0(\zeta_l)\} \times\exp(\zeta_l 0^+)+\Omega'\{G_0\}+O(G_{\mathrm{osc}}^2). \quad (9)$$

In (9),

$$S_0'(\zeta_l)=1/[\zeta_l-\epsilon-G_0(\zeta_l)]. \quad (10)$$

Again, consistent with our assumptions, we can drop the last term in (9). This is because it is $O[(\omega/\mu)^3]$. The rest, as we shall see, gives rise to conventional DHVA oscillations in Ω, which are of order of $(\omega/\mu)^{\frac{3}{2}}$. [See, for example, reference 5, Eq. (2.17).] Therefore, the leading term of the DHVA oscillations is contained in

$$\Omega=\frac{-1}{\beta}\sum_l \mathrm{Tr}\{\ln[\epsilon+G_0(\zeta_l)-\zeta_l] +S_0'(\zeta_l)G_0(\zeta_l)\}\exp(\zeta_l 0^+)+\Omega'(G_0). \quad (11)$$

We next have to consider the oscillatory contribution of Ω' to (11). This can only come from summations in the intermediate states over the propagators S_0'. Now these oscillations are a nonanalytic type of behavior in magnetic field, the argument of the trigonometric functions containing $1/H$.[5] Therefore, they can only come from places where some $S_0'(\zeta_l)$ becomes a singular matrix. Just as in the case of a simple diagonal propagator this only happens when ζ_l is very near μ. $G_0(\zeta_l)$ can be resolved into an Hermitian and anti-Hermitian part, the anti-Hermitian part being positive definite and approaching zero as $(\zeta_l-\mu)^2$ for ζ_l near μ.[6] This means that except for ζ_l near μ, $\zeta_l-\epsilon-G_0(\zeta_l)$ cannot vanish and S_0' cannot be singular. Therefore, the contribution of Ω' to the oscillatory behavior of Ω only comes from a little region of each line close to μ. Since we are interested in the leading term of the oscillatory behavior, it is obtained by taking this contribution in any diagram once from each line and ignoring it from the rest of the lines in a diagram. Therefore, the oscillatory behavior of Ω' is the same as that of[7]

$$\mathrm{Tr}\left\{\frac{1}{\beta}\sum_l S_0'(\zeta_l)D(\zeta_l)\exp(\zeta_l 0^+)\right\}, \quad (12)$$

where $D(\zeta_l)$ is the matrix we get by opening a single line

[6] These results on $G(\zeta_l)$ follow in almost identical fashion to the corresponding ones[3] for a simple propagator.

[7] The factor $\exp(\zeta_l 0^+)$ in (12) is only necessary for those contributions which lead to a $D(\zeta_l)$ independent of ζ_l. It comes because in those diagrams there is the prescription in the original formalism that for a disconnected propagator (not connected to others by ζ_l summations), we must multiply by $\exp(\zeta_l 0^+)$.

in all possible ways for the closed-linked skeleton diagrams, dropping all oscillatory contributions. But this is just $G_0(\zeta_l)$. Therefore, the oscillatory part of $\Omega'\{G_0\}$ is contained in

$$\mathrm{Tr}\left\{\frac{1}{\beta}\sum_l S_0'(\zeta_l)G_0(\zeta_l)\exp(\zeta_l 0^+)\right\}. \tag{13}$$

Combining (13) with (11), we see that

$$\Omega_{\text{osc part}}=\left[-\frac{1}{\beta}\mathrm{Tr}\sum_l\{\ln[\epsilon+G_0(\zeta_l)-\zeta_l]\}\times\exp(\zeta_l 0^+)\right]_{\text{osc part}}. \tag{14}$$

The reasoning which leads from (11) to (14) is, incidentally, formally identical with that which leads to the expression (I.44) used to compute the first term in the temperature dependence of Ω.

We shall drop the notation "osc part" from (14) from now on, it being understood that the equation is only valid for the computation of the oscillatory part of Ω.

Just as in I, let us introduce the characteristic values of the matrix $\epsilon+G_0(\zeta_l)$, which we shall call $L_r(\zeta_l)$. Then (14) becomes

$$\Omega=-\frac{1}{\beta}\sum_r\sum_l\exp(\zeta_l 0^+)\ln[L_r(\zeta_l)-\zeta_l]. \tag{15}$$

By means of the usual argument of LW (Appendix A), we may write (15) as

$$\Omega=-\sum_r\int_\infty^\infty\frac{dx}{e^{\beta(x-\mu)}+1}\frac{1}{2\pi i}\{\ln[Q_r(x)-x+iJ_r(x)]-\ln[Q_r(x)-x-iJ_r(x)]\}, \tag{16}$$

where

$$\lim_{\eta\to 0+}L_r(x-i\eta)\equiv Q_r(x)+iJ_r(x). \tag{17}$$

$J_r(x)$ is non-negative and behaves like $(x-\mu)^2$ as x approaches μ. Therefore, in the neighborhood of μ (which is the part we need for the oscillatory behavior) $J_r(x)$ approaches zero, and we may write from (I.49)

$$\Omega=-\sum_r\int_{-\infty}^\infty\frac{dx}{e^{\beta(x-\mu)}+1}\theta(x-Q_r(x)), \tag{18}$$

where

$$\theta(t)=1,\quad t>0;\qquad =0,\quad t<0. \tag{19}$$

Let us introduce as usual the "single-particle excitation energies" E_r by

$$E_r-Q_r(E_r)=0. \tag{20}$$

Then

$$\theta(x-Q_r(x))=\theta(x-E_r), \tag{21}$$

and (18) becomes

$$\Omega=-\sum_r\int_r^\infty\frac{dx}{e^{\beta(x-\mu)}+1}=-\frac{1}{\beta}\sum_r\ln(1+e^{\beta(\mu-E_r)}). \tag{22}$$

The expression (22) is exactly the thermodynamic potential for a collection of independent fermions with the energy levels E_r.[8] It only remains to investigate these levels for our case.

III. SINGLE-PARTICLE EXCITATION ENERGIES IN THE PRESENCE OF A MAGNETIC FIELD

To study the effect of an external magnetic field on the single-particle excitation energies, it is necessary to study the field dependence of the propagator. To do this we shall make use of the gauge invariance of the entire theory. That is, if the vector potential $\mathbf{A}$ is replaced by $\mathbf{A}'$, where

$$\mathbf{A}'=\mathbf{A}+\nabla\chi \tag{23}$$

(χ being any scalar function of position), all physical results are unchanged. In particular this means that the energy levels E_r must be invariant under the transformation (23). This in turn means that the "Hamiltonian" $\epsilon+G_0(\zeta_l)$, from which the E_r are computed, must be a "gauge-invariant" operator in the same sense as any single-particle Hamiltonian for a particle in a magnetic field. We now make this statement more precise and prove it.

It is convenient to work in the coordinate representation. For this representation the total Hamiltonian of the system takes the form

$$\mathfrak{IC}=\int d\mathbf{x}\,\psi_\sigma^\dagger(\mathbf{x})\epsilon\psi_\sigma(\mathbf{x})+\frac{1}{2}\int d\mathbf{x}d\mathbf{x}'\,\psi_\sigma^\dagger(\mathbf{x})\psi_{\sigma'}^\dagger(\mathbf{x}')\times v_{\sigma\sigma'\sigma''\sigma'''}(\mathbf{x},\mathbf{x}')\psi_{\sigma''}(\mathbf{x}')\psi_{\sigma'''}(\mathbf{x}). \tag{24}$$

Here repeated spin indices $(\sigma,\sigma',\sigma'',\sigma''')$ are summed over. $v_{\sigma\sigma'\sigma''\sigma'''}(\mathbf{x},\mathbf{x}')$ is the interaction between a pair of particles (assumed velocity-independent for simplicity of writing). ϵ is the Hamiltonian of the individual particles. For the case of a particle of mass m, charge e, magnetic moment μ_B, spin $\frac{1}{2}$, moving in an external periodic potential U and external magnetic field $\mathbf{H}$, we have

$$\epsilon=\frac{[\mathbf{p}-(e/c)\mathbf{A}]^2}{2m}+U-\mu_B\mathbf{H}\cdot\boldsymbol{\sigma}, \tag{25}$$

where $\boldsymbol{\sigma}$ is the Pauli spin matrix vector.

Next we need the matrix propagator in the coordinate representation. That is, we need to investigate $S'(\mathbf{x}\sigma,\mathbf{x}'\sigma';\zeta_l)$. As is convenient for such general dis-

[8] We emphasize again that expression (22) is only valid for calculating the oscillatory part of Ω.

cussions, we write this as[9]

$$S'(\mathbf{x}\sigma,\mathbf{x}'\sigma';\zeta_l)=\int^{\beta} e^{-\zeta_l u}S'(\mathbf{x}\sigma,\mathbf{x}'\sigma';u)du, \tag{26}$$

$$S'(\mathbf{x}\sigma,\mathbf{x}'\sigma';u)=\mathrm{Tr}\{\exp[\beta(\Omega-\mathfrak{K}+\mu N)] \times T(\psi_{\sigma'}{}^{\dagger}(\mathbf{x}',u)\psi_{\sigma}(\mathbf{x}))\}, \tag{27}$$

where

$$T(\psi_{\sigma'}{}^{\dagger}(\mathbf{x}';u)\psi_{\sigma}(\mathbf{x}))=\psi_{\sigma'}{}^{\dagger}(\mathbf{x}',u)\psi_{\sigma}(\mathbf{x}), \quad u>0$$
$$=-\psi_{\sigma}(\mathbf{x})\psi_{\sigma'}{}^{\dagger}(\mathbf{x}',u), \quad u<0, \tag{28}$$

and

$$\psi_{\sigma'}{}^{\dagger}(\mathbf{x}',u)=\exp(\mathfrak{K}u)\psi_{\sigma'}{}^{\dagger}(x')\exp(-\mathfrak{K}u). \tag{29}$$

Under the transformation (23), H goes over into H'. As one sees immediately, H' is given by the same expression (24) as H, where we have replaced $\psi_{\sigma}(\mathbf{x})$ by

$$\psi_{\sigma}{}'(\mathbf{x})=e^{-i(e/c)\chi(\mathbf{x})}\psi_{\sigma}(\mathbf{x}). \tag{30}$$

It may be verified easily that ψ' and ψ satisfy the same commutation rules so that they are related by a canonical transformation B:

$$\psi_{\sigma}{}'(\mathbf{x})=B\psi_{\sigma}(x)B^{-1},$$
$$\mathfrak{K}'=B\mathfrak{K}B^{-1}. \tag{31}$$

Therefore we have

$$[S'(\mathbf{x}\sigma,\mathbf{x}'\sigma';u)]_{\mathrm{A}+\nabla\chi}$$
$$=\mathrm{Tr}\{\exp[\beta(\Omega-\mathfrak{K}'+\mu N)] \times T(\exp(\mathfrak{K}'u)\psi_{\sigma'}{}^{\dagger}(\mathbf{x}')\exp(-\mathfrak{K}'u)\psi_{\sigma}(\mathbf{x}))\}$$
$$=\mathrm{Tr}\{\exp[\beta(\Omega-\mathfrak{K}-\mu N)]T(\exp(\mathfrak{K}u)B^{-1}\psi_{\sigma'}{}^{\dagger}(\mathbf{x}')B \times\exp(-\mathfrak{K}u)B^{-1}\psi_{\sigma}(\mathbf{x})B)\}. \tag{32}$$

However, from (31) and (30) we have

$$B^{-1}\psi_{\sigma}(\mathbf{x})B=e^{i(e/c)\chi(\mathbf{x})}\psi_{\sigma}(\mathbf{x}), \tag{33}$$

$$B^{-1}\psi_{\sigma'}{}^{\dagger}(\mathbf{x}')B=e^{-i(e/c)\chi(\mathbf{x}')}\psi_{\sigma'}{}^{\dagger}(\mathbf{x}'). \tag{34}$$

Therefore (32) becomes

$$[S'(\mathbf{x}\sigma,\mathbf{x}'\sigma';u)]_{\mathrm{A}+\nabla\chi} =e^{i(e/c)[\chi(\mathbf{x})-\chi(\mathbf{x}')]}[S'(\mathbf{x}\sigma,\mathbf{x}'\sigma';u]_{\mathrm{A}}, \tag{35}$$

or

$$[S'(\mathbf{x}\sigma,\mathbf{x}'\sigma';\zeta_l)]_{\mathrm{A}+\nabla\chi} =e^{i(e/c)[\chi(\mathbf{x})-\chi(\mathbf{x}')]}[S'(\mathbf{x}\sigma,\mathbf{x}'\sigma';\zeta_l)]_{\mathrm{A}}. \tag{36}$$

Now suppose we view S' in operator form expressed somehow as a function of the operators $\mathbf{p}$, $\mathbf{r}$ and of course the spin variables $\boldsymbol{\sigma}$. Write

$$[S']_{\mathrm{A}}=S'(\mathbf{p},\mathbf{r},\boldsymbol{\sigma};\mathbf{A},\mathbf{H}), \tag{37}$$

$$[S']_{\mathrm{A}+\nabla\chi}=S'(\mathbf{p},\mathbf{r},\boldsymbol{\sigma};\mathbf{A}+\nabla\chi,\mathfrak{K}). \tag{38}$$

(36) tells us that

$$S'(\mathbf{p},\mathbf{r},\boldsymbol{\sigma};\mathbf{A}+\nabla\chi,\mathbf{H}) =e^{i(e/c)\chi(\mathbf{r})}S'(\mathbf{p},\mathbf{r},\boldsymbol{\sigma};\mathbf{A},\mathbf{H})e^{-i(e/c)\chi(\mathbf{r})}$$
$$=S'(\mathbf{p}-(e/c)\nabla\chi,\mathbf{r},\boldsymbol{\sigma};\mathbf{A},\mathbf{H}). \tag{39}$$

[9] This representation, which is well known from field theory, has already been used in reference 3 to discuss the analytic properties of the propagator.

Since the different components of $\mathbf{p}-(e/c)\nabla\chi$ commute, there is no ambiguity about the order of the factors in (39).

We can only satisfy (39) identically for arbitrary $\mathbf{A}$ if the vector potential only enters in the combination $\mathbf{p}-(e/c)\mathbf{A}$. That is, we have shown from gauge invariance that S' has the form

$$S'=S'(\mathbf{p}-(e/c)\mathbf{A},\mathbf{r},\boldsymbol{\sigma};\mathbf{H}). \tag{40}$$

Since the different components of $\mathbf{p}-(e/c)\mathbf{A}$ do not commute with each other, there is some ambiguity in the order of the factors occurring in (40). The order of these factors can be fixed for example by imagining (39) expanded in power series in the components of $\mathbf{p}$, $\mathbf{A}$, and $\nabla\chi$. Then one sees easily that (40) means that if we expand in components of $\mathbf{p}-(e/c)\mathbf{A}$ we have to symmetrize completely our result with respect to all these components.

While this result is not at all surprising, we have felt it important to exhibit it in detail for one reason. If we replaced e in (40) by some other number e^*, S' would still have a formal gauge-invariance property, but the single-particle excitations would behave as if they had an effective charge e^* instead of the original charge e. It has often been suggested that this might be the case.[10] However, our method of connecting the gauge invariance of S' with that of the original Hamiltonian shows that in fact, as far as the response to an external magnetic field is concerned, it is e which comes into (40) and not some e^*. That is, the charge of the elementary excitations is the same as that of the original particles.

Actually, if the metal has a magnetic permeability ϵ_m, the vector potential in the medium should be multiplied by a factor ϵ_m. Since we have an exact many-body theory these effects should be included automatically if the calculation is done correctly. It is lost in (40) because we have assumed in making the estimates that led to our results, that the interaction between the particles is short-ranged. The permeability factor comes from the long-range magnetic forces between the particles.[11] This error is completely negligible, ϵ_m differing from unity by about 10^{-5} for common metals.

Since ϵ has the form (40), it follows that the proper self-energy part does also

$$G(\zeta_l)=G(\mathbf{p}-(e/c)\mathbf{A},\mathbf{r},\boldsymbol{\sigma};\mathbf{H};\zeta_l). \tag{41}$$

According to (17) and (20), what we need to compute the single-particle excitation energies are the characteristic values $Q_r(\xi)$ of the "effective Hamiltonian" $h(\xi)$ defined by

$$h(\xi)=\epsilon+K(\xi), \tag{42}$$

[10] See, for example, the articles by E. A. Stern and L. M. Falicov in *The Fermi Surface*, edited by W. A. Harrison and M. B. Webb (John Wiley & Sons, Inc., New York, 1960).

[11] V. Ambegaokar, doctoral dissertation, Carnegie Institute of Technology, March, 1960 (unpublished). See also A. Klein, Phys. Rev. **115**, 1136 (1959).

where

$$\lim_{\eta\to 0+} G_0(\xi-i\eta)=K(\xi)+iJ(\xi), \tag{43}$$

K and J both being Hermitian. From (25) and (41), this has the form

$$h=h(\mathbf{p}-(e/c)\mathbf{A},\ \mathbf{r},\ \boldsymbol{\sigma};\ \mathbf{H};\ \xi). \tag{44}$$

Now the inclusion of the spin splits otherwise degenerate levels by small amounts proportional to $\mu_B H$. This leads[5] to a change in the value of the phase of the DHVA oscillations, but does not affect their period. The correct calculation of this phase is in fact quite complicated, and we shall not go into it here. We wish only to point out that many-body effects do influence it, and its value is not given by the simple expression of Lifshitz and Kosevich, which assumed that the spin only enters the quasi-particle energy through a factor $-\mu_B\mathbf{H}\cdot\boldsymbol{\sigma}$.

Dropping the spin dependence of (44), we may write

$$h=h(\mathbf{p}-(e/c)\mathbf{A},\ \mathbf{r},\ \mathbf{H};\ \xi). \tag{45}$$

We now expand (45) in powers of the $\mathbf{H}$ which appears explicitly in it.

$$h=h_0(\mathbf{p}-(e/c)\mathbf{A},\ \mathbf{r};\ \xi) +H_\alpha L_\alpha(\mathbf{p}-(e/c)\mathbf{A},\ \mathbf{r};\ \xi)+O(H^2), \tag{46}$$

where we sum on the repeated α indices over the Cartesian components of $\mathbf{H}$. By time-reversal arguments, the term linear in $\mathbf{H}$ has no expectation value linear in $\mathbf{H}$ for eigenstates of h_0. Therefore up to terms of order H^2 we can use the first term of (46) to compute the characteristic values. We can actually drop the H^2 terms since, in the sense of this paper, they give corrections to the DHVA period of the order $(\omega/\mu)^2$ and to the phase of order ω/μ. Therefore we have the result that the characteristic values of h can be obtained with sufficient accuracy for DHVA purposes from

$$h=h_0(\mathbf{p}-(e/c)\mathbf{A},\ \mathbf{r};\ \xi). \tag{47}$$

If $\mathbf{A}$ is zero, h_0 is just the Hamiltonian which is used to compute the single-particle excitation energies for the band case without external field. That is, if we put

$$h_0(\mathbf{p},\mathbf{r};\ \xi)\phi_{\nu\mathbf{k}}=Q_\nu(\mathbf{k};\ \xi)\phi_{\nu\mathbf{k}} \tag{48}$$

(where ν is a band index and $\mathbf{k}$ the quasi-momentum of the excitations), then the single-particle excitation energies $E_\nu(\mathbf{k})$ are given by

$$E_\nu(\mathbf{k})-Q_\nu(\mathbf{k};\ E_\nu(\mathbf{k}))=0. \tag{49}$$

The Fermi surface of the metal was shown to be[1] the collection of those surfaces for which

$$E_\nu(\mathbf{k})=\mu. \tag{50}$$

To find the excitation energies E_r in the magnetic field, we must find the characteristic values $Q_r(\xi)$ of h_0

$$h_0(\mathbf{p}-(e/c)\mathbf{A},\ \mathbf{r};\ \xi)\psi_r=Q_r(\xi)\psi_r, \tag{51}$$

and then use (20).

Now it is well known[12] how to obtain the characteristic values of (51) from those of (48) with sufficient accuracy for the DHVA effect. The $Q_r(\xi)$ are obtained from the $Q_\nu(\mathbf{k};\ \xi)$ by using $Q_\nu(\mathbf{p}-(e/c)\mathbf{A};\ \xi)$ as the Hamiltonian [symmetrized with respect to the components of $\mathbf{p}-(e/c)\mathbf{A}$ in the same sense as in the discussion immediately following (40)], and using the WKB approximation to obtain the levels. If the field is in the z direction, then the equation for these levels is[5,12]

$$A_\nu(Q_r(\xi),k_z;\ \xi)=2\pi(n+\tfrac{1}{2})(eH/c), \tag{52}$$

where n is an integer and r stands for the index triple ν, n, k_z. The quantity $A_\nu(Q,k_z;\ \xi)$ is the cross-sectional area of the curve given by the intersection of $Q_\nu(\mathbf{k};\ \xi)=Q$ and the plane k_z fixed. Using (20), E_r is then obtained from

$$A_\nu(E_r,k_z;\ E_r)=2\pi(n+\tfrac{1}{2})(eH/c). \tag{53}$$

Now consider the levels which we would obtain if we had used $E_\nu(\mathbf{p}-(e/c)\mathbf{A})$ as the Hamiltonian. Call these E_r'. From the WKB procedure these levels are given by

$$A_\nu'(E_r',k_z)=2\pi(n+\tfrac{1}{2})(eH/c), \tag{54}$$

where $A_\nu'(E,k_z)$ is the cross-sectional area of the curve given by the intersection of $E_\nu(\mathbf{k})=E$ and the plane k_z fixed.

From its definition, $A_\nu(E,k_z;\ E)$ is the area of curve given by the intersection of $Q_\nu(\mathbf{k};\ E)=E$ with the plane k_z constant. However, from the definition (49) of $E_\nu(k)$, this is the same as the intersection of $E_\nu(k)=E$ with the plane k_z constant. Therefore,

$$A_\nu'(E,k_z)=A_\nu(E,k_z;\ E), \tag{55}$$

or

$$E_r'=E_r. \tag{56}$$

This means that the levels E_r can be computed in the usual way of Lifshitz and Kosevich, using the single-particle excitation energies as if they were real independent particles with charge e and kinetic energy $E_\nu(\mathbf{k})$. In conjunction with (22) this means that the DHVA effect (apart from the phase of the oscillations) in all equilibrium properties (magnetization, heat capacity, etc.) is exactly what one usually computes on the single-particle basis, except that the true single-particle excitation energies must be used, and the true Fermi surface is what determines the period of the oscillations.

[12] W. Kohn, Phys. Rev. **115**, 1460 (1959). Kohn only considers the simple case where the Hamiltonian without field is of the form $p^2/2m+U$. It is not difficult to generalize his argument to an arbitrary periodic Hamiltonian. See also W. Kohn, Proc. Phys. Soc. (London) **72**, 1147 (1958), for a summary of the consequences of the application of these results to the DHVA effect. This prescription is only valid with sufficient accuracy for the DHVA problem, if there is a center of symmetry present. We shall assume this to be the case. Even if a center of symmetry is not present, this formula is still good enough to give the period of the oscillations correctly, but not the phase.

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APPENDIX A. THE FIRST-ORDER PROPER SELF-ENERGY PART IN A MAGNETIC FIELD

In this Appendix we give an explicit calculation of the field dependence of G, to the first order in the interaction. For simplicity we omit the spin and the periodic lattice, and take an isotropic interaction. The first-order proper self-energy part $G_{rr'}{}^{(1)}$ is given by (see I, Appendix A)

$$G_{rr'}{}^{(1)}=\sum_s f_s{}^-\{(rs|v|r's)-(rs|v|sr')\}, \tag{A.1}$$

$$f_s{}^-\equiv\frac{1}{e^{\beta(\epsilon_s-\mu)}+1}, \tag{A.2}$$

$$(r_1r_2|v|r_3r_4)\equiv\int\psi_{r_1}{}^*(\mathbf{x}_1)\psi_{r_2}{}^*(\mathbf{x}_2)v(\mathbf{x}_1,\mathbf{x}_2)\times\psi_{r_3}(\mathbf{x}_1)\psi_{r_4}(\mathbf{x}_2)d\mathbf{x}_1d\mathbf{x}_2. \tag{A.3}$$

Here the ψ_r,ϵ_r are the eigenfunctions and eigenvalues, respectively, of the unperturbed single-particle Hamiltonian; $v(\mathbf{x}_1,\mathbf{x}_2)$ the interaction between a pair of particles. We take as the unperturbed single-particle Hamiltonian (ϵ)

$$\epsilon=\tfrac{1}{2}[\mathbf{p}-(e/c)\mathbf{A}]^2, \tag{A.4}$$

where we have chosen units so that the mass of the particles is unity. We have

$$\epsilon\psi_r=\epsilon_r\psi_r. \tag{A.5}$$

Inserting (A.3) into (A.1) we may write for the matrix $G^{(1)}(1)$ in the coordinate representation

$$G^{(1)}(1)=\int d\mathbf{x}_2\, v(\mathbf{x}_1,\mathbf{x}_2)[\rho(22)-\rho(21)P_{12}], \tag{A.6}$$

where

$$\rho(21)\equiv\sum_r f_r{}^-\psi_r{}^*(\mathbf{x}_2)\psi_r(\mathbf{x}_1), \tag{A.7}$$

and P_{12} is the exchange operator

$$P_{12}\phi(\mathbf{x}_1)=\phi(\mathbf{x}_2). \tag{A.8}$$

This operator may be written formally as

$$P_{12}=e^{i(\mathbf{x}_2-\mathbf{x}_1)\cdot\mathbf{p}_1}, \tag{A.9}$$

it being understood that in the expansion the $\mathbf{p}_1$ is not to differentiate the $\mathbf{x}_1$ in the exponent. This form will be of use later on.

We must next calculate $\rho(21)$. This is done most conveniently as follows. Write

$$\rho(21)=\sum_r\psi_r{}^*(\mathbf{x}_2)\frac{1}{e^{\beta(\epsilon_1-\mu)}+1}\psi_r(\mathbf{x}_1). \tag{A.10}$$

We make use of the identity

$$\frac{1}{e^x+1}=\frac{1}{2\pi i}\int_{-i\infty+c}^{i\infty+c}dt\,\frac{e^{-tx}}{(1/\pi)\sin\pi t},\quad(0<c<1), \tag{A.11}$$

which is easily proved by closing the contour to the left if x is less than zero and to the right if x is greater than zero. With (A.11), we may write $\rho(21)$ as

$$\rho(21)=\frac{1}{2\pi i}\int_{-i\infty+c}^{i\infty+c}\frac{dt}{(1/\pi)\sin\pi t}e^{+t\beta\mu}Q(\mathbf{x}_2,\mathbf{x}_1;t\beta), \tag{A.12}$$

where

$$Q(\mathbf{x}_2,\mathbf{x}_1;\gamma)\equiv\sum_r\psi_r{}^*(\mathbf{x}_2)e^{-\gamma\epsilon_1}\psi_r(\mathbf{x}_1). \tag{A.13}$$

The reason for writing ρ in this form is that Q is easy to calculate exactly for the Hamiltonian (A.4).[13]

Choosing the Landau gauge

$$\mathbf{A}=(-Hy,0,0), \tag{A.14}$$

the result is

$$Q(\mathbf{x}_2,\mathbf{x}_1;\gamma)=\exp(i\omega(y_2+y_1)(x_2-x_1)/2)\times F(\mathbf{x}_2-\mathbf{x}_1;\omega;\gamma), \tag{A.15}$$

$$\omega\equiv eH/c,$$

$$F(\mathbf{r};\omega;\gamma)=\left(\frac{1}{2\pi\gamma}\right)^{\frac{1}{2}}\left(\frac{\omega}{4\pi\sinh(\omega\gamma/2)}\right)\times\exp-\left\{\frac{\omega}{4}\coth\left(\frac{\omega\gamma}{2}\right)(x^2+y^2)+\frac{1}{2\gamma}z^2\right\}. \tag{A.16}$$

In (A.16), $\gamma^{\frac{1}{2}}$ means that branch of the function which is positive on the real axis.

From (A.12) we have

$$\rho(21)=\exp(i\omega(y_2+y_1)(x_2-x_1)/2)g(\mathbf{x}_2-\mathbf{x}_1;\omega), \tag{A.17}$$

$$g(\mathbf{r};\omega)=\frac{1}{2\pi i}\int_{-i\infty+c}^{i\infty+c}\frac{dt}{(1/\pi)\sin\pi t}e^{t\beta\mu}F(\mathbf{r};\omega;t\beta). \tag{A.18}$$

Using (A.17), (A.6) becomes

$$G^{(1)}(1)=\int d\mathbf{x}_2\, v(|\mathbf{x}_2-\mathbf{x}_1|)\times\left[g(0;\omega)-\exp\left(i\omega\frac{(y_2+y_1)(x_2-x_1)}{2}\right)\times g(\mathbf{x}_2-\mathbf{x}_1;\omega)P_{12}\right]. \tag{A.19}$$

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[13] E. H. Sondheimer and A. H. Wilson, Proc. Roy. Soc. (London) **A210**, 173 (1951). See also A. H. Wilson, *Theory of Metals* (Cambridge University Press, New York, 1958), pp. 160–170. Wilson uses a slightly different gauge than we do. It is easy to see that for any vector potential linear in the coordinates, the F in (A.15) is unchanged and the phase factor in front becomes

$$\exp\left\{\frac{ie}{2c}(\mathbf{x}_1+\mathbf{x}_2)\cdot[\mathbf{A}(\mathbf{x}_1-\mathbf{x}_2)-\mathbf{H}\times(\mathbf{x}_1-\mathbf{x}_2)]\right\}.$$

Changing the integration variable from $\mathbf{x}_2$ to $\mathbf{r}=\mathbf{x}_2-\mathbf{x}_1$, and using (A.9), this becomes

$$G^{(1)}(1)=\int d\mathbf{r}\, v(r)[g(0;\omega) - g(\mathbf{r};\omega)e^{i\omega x(y_1+y/2)}e^{i\mathbf{r}\cdot\mathbf{p}_1}]. \quad \text{(A.20)}$$

By means of the elementary operator identity[14]

$$e^{A+B}=e^Ae^Be^{-\frac{1}{2}(A,B)} \quad \text{(A.21)}$$

[which is true as long as the commutator (A,B) commutes with both A and B], we have

$$e^{i\omega x(y_1+y/2)}e^{i\mathbf{r}\cdot\mathbf{p}_1}=\exp\left[i\mathbf{r}\cdot\left(\mathbf{p}_1-\frac{e}{c}\mathbf{A}_1\right)\right]. \quad \text{(A.22)}$$

Therefore

$$G^{(1)}(1)=\int d\mathbf{r}\, v(\mathbf{r})\left\{g(0;\omega)-g(r;\omega) \times\exp\left[i\mathbf{r}\cdot\left(\mathbf{p}_1-\frac{e}{c}\mathbf{A}_1\right)\right]\right\}. \quad \text{(A.23)}$$

Thus we have verified in detail the general gauge invariance property (41) for this simple case.

It now remains to calculate $g(\mathbf{r};\omega)$. As one easily sees, the contour in (A.18) may be closed by a very large semicircle to the left, without changing the value of the integral. The singularities of the integrand within the resulting contour are on the negative real axis (which is also a branch cut) and, in addition, at the points

$$t_l=(2\pi il/\beta\omega), \quad l=\pm1,\pm2,\cdots\pm\infty, \quad \text{(A.24)}$$

where $\sinh(\omega\beta t/2)$ vanishes. Therefore, we may write

$$g(\mathbf{r};\omega)=g_0(\mathbf{r};\omega)+g_1(\mathbf{r};\omega), \quad \text{(A.25)}$$

$$g_0(\mathbf{r};\omega)=\frac{1}{2\pi i}\int_C\frac{dt}{(1/\pi)\sin\pi t}e^{t\beta\mu}F(\mathbf{r};\omega;t\beta), \quad \text{(A.26)}$$

where C is a contour which proceeds counter clockwise around the negative real axis, and infinitesimally close to it.

$$g_1(\mathbf{r};\omega)=\sum_{l=-\infty}^{\infty}{}'\frac{1}{2\pi i}\int_{C_l}\frac{dt}{(1/\pi)\sin\pi t}e^{t\beta\mu}F(\mathbf{r};\omega;tp), \quad \text{(A.27)}$$

where C_l is a contour consisting of a very small circle proceeding counterclockwise around the point t_l. The prime on the summation indicates that $l=0$ is excluded, the origin being contained inside the contour C.

We shall evaluate these expressions in the usual limit of interest for the DHVA oscillations: ω, $1/\beta\ll\mu$, but $\omega\beta$ of the order of unity. Further, we need to know the order of magnitude of $\mathbf{r}$, which also comes into (A.18). For a short-range potential this is limited [see (A.23)] by the range of the potential. Roughly speaking, for typical metals the screened Coulomb potential has a cutoff length comparable to the reciprocal Fermi momentum. Therefore we shall assume

$$2\mu r^2\sim1 \quad \text{(A.28)}$$

(in our units an energy is a reciprocal length squared). Under these circumstances g_0 and g_1 are easily obtained.

First consider g_0. Let us change the integration variable from t to α,

$$t=\alpha/\beta\mu. \quad \text{(A.29)}$$

Because of the factor e^α now occurring in (A.26) and the fact that the integration contour runs along the negative α direction, this integral gets cut off for α of order of unity. Therefore, we can expand the integrand in (A.26). As one easily sees,

$$F(\mathbf{r};\omega;\alpha/\mu)=\frac{\mu^{\frac{3}{2}}}{(2\pi)^{\frac{3}{2}}}\frac{\exp(-w^2/4\alpha)}{\alpha^{\frac{3}{2}}}+O[(\omega/\mu)^2], \quad w^2\equiv2\mu r^2, \quad \text{(A.30)}$$

on using (A.28) as well as the usual DHVA conditions (4).

Similarly we get for the entire integral in (A.26)

$$g_0(\mathbf{r};\omega)=\frac{\mu^{\frac{3}{2}}}{(2\pi)^{\frac{3}{2}}}\frac{1}{2\pi i} \times\int_C\frac{d\alpha}{\alpha^{\frac{3}{2}}}\exp\left(\alpha-\frac{w^2}{4\alpha}\right)\alpha+O(\omega/\mu)^2. \quad \text{(A.31)}$$

This well-known integral may be done at once,[15] yielding

$$g_0(r;\omega)=\mu^{\frac{3}{2}}\frac{\sqrt{2}}{\pi^2}\frac{\sin w-w\cos w}{w^3}+O[(\omega/\mu)^2]. \quad \text{(A.32)}$$

The leading term here (the only one we have evaluated) is of course just what we'd get if no magnetic field were present, which may be verified immediately by starting with the zero-field case.

The term g_1 is a little more complicated to evaluate in the lowest order for which it exists. Putting on the lth contour of (A.27)

$$t=t_l+\gamma'/\beta, \quad \text{(A.33)}$$

F becomes

$$F=\frac{\omega}{2(2\pi)^{\frac{3}{2}}(\beta t_l+\gamma')^{\frac{1}{2}}}\frac{(-1)^l}{\sinh(\omega\gamma'/2)} \times\exp-\left\{\frac{\omega}{4}\coth\left(\frac{\omega\gamma'}{2}\right)(x^2+y^2)+\frac{z^2}{2(\beta t_l+\gamma')}\right\}. \quad \text{(A.34)}$$

[14] This can be verified, for example, by direct power series expansion of both sides of the equation.

[15] W. Magnus and F. Oberhettinger, *Special Functions of Mathematical Physics* (Chelsea Publishing Company, New York, 1949), p. 28.

On the contour C_l we are integrating over a small circle around the origin in γ'. It is not difficult to see that the leading term comes from expanding in γ', higher order corrections to the term we give being $O(\omega/\mu)$;

$$F=\frac{1}{(2\pi)^{\frac{3}{2}}(\beta t_l)^{\frac{1}{2}}}\frac{(-1)^l}{\gamma'}\times\exp\left[-\left(\frac{x^2+y^2}{2\gamma'}\right)\right]+O(\omega/\mu). \quad (A.35)$$

Proceeding similarly for the rest of the integrand, we obtain finally

$$g_1(\mathbf{r};\omega)=\frac{\pi}{(2\pi)^{\frac{3}{2}}\beta}\sum_{l=-\infty}^{\infty}{}'\frac{(-1)^l e^{\beta\mu t_l}}{(\beta t_l)^{\frac{3}{2}}\sin\pi t_l}\frac{1}{2\pi i}\times\oint\frac{\exp\{\gamma'\mu-(x^2+y^2)/2\gamma'\}}{\gamma'}d\gamma'. \quad (A.36)$$

The last integral is again well known.[15] Substituting its value and that of t_l, we finally obtain (up to correction terms of order ω/μ)

$$g_1(\mathbf{r};\omega)=\frac{\omega^{\frac{3}{2}}}{2\pi}\sum_{l=1}^{\infty}\frac{(-1)^l\sin(2\pi l\mu/\omega-\pi/4)}{l^{\frac{1}{2}}\beta\omega\sinh(2\pi^2 l/\beta\omega)}\times J_0\{[2\mu(x^2+y^2)]^{\frac{1}{2}}\}. \quad (A.37)$$

When g_1 is put into (A.23) it will yield the oscillatory terms in the proper self-energy part. Comparing g_0 from (A.32) with g_1, we see that g_1/g_0 is of the order of $(\omega/\mu)^{\frac{3}{2}}$, which is the estimate we used in obtaining the general formula for the DHVA oscillations in the thermodynamic potential. It is easy to trace down the origin of the $\omega^{\frac{3}{2}}$ dependence of g_1: it arises from the f_s^- factor in (A.1). This same kind of dependence comes in higher order skeleton diagrams from the sums on the true propagators, for ζ_l near μ, and therefore it is easy to see that this $\omega^{\frac{3}{2}}$ dependence is quite general.

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Dielectric Constant, Density, Expansion Coefficient, and Entropy of Liquid He^3 Under Pressure Below 1°K*†

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By measuring the resonant frequency of an LC circuit containing a capacitor filled with liquid He^3, the dielectric constant of the liquid was measured from 0.14 to 1°K at several pressures from 0.2 to 29.5 atmospheres. From these measurements the density, expansion coefficient at constant pressure, and the change in entropy on compression from saturated vapor pressure to higher pressures were determined. α_p was found to be negative and, hence, $(\partial S/\partial P)_T$ positive for all pressures below a certain temperature which increased monotonically with pressure, confirming behavior found by Brewer and Daunt. A minimum in the melting curve of He^3 was found at $T=0.32\pm0.01$°K and $p=29.1\pm0.1$ atm. The results are compared with those obtained by other methods.

I. INTRODUCTION

THE present experiment is an outgrowth of an earlier set of measurements on the heat transport properties of liquid He^3 in which it was found from the convection behavior that a maximum in the density occurs at 0.5°K for a pressure of $\frac{2}{3}$ atmosphere.[1]

In this paper we report experimental measurements of the density, ρ, the thermal expansion coefficient at constant pressure, α_p, and entropy of compression of liquid He^3 at temperatures from 0.14 to 1.0°K and at pressures from 0.2 to 29 atmospheres. Because the changes in density below 1°K are small, a sensitive method of measurement was required. The limited amounts of He^3 available likewise restricted the size of the liquid sample. Both of these requirements were satisfactorily met in a measurement of the dielectric constant, ϵ, of the liquid as described in Sec. II. The density of the liquid was found from ϵ, using the Clausius-Mossotti relation,

$$\frac{\epsilon-1}{\epsilon+2}\frac{M}{\rho}=\frac{4\pi}{3}A, \quad (1)$$

where M is the molecular weight and A is the molar polarizability. $\alpha_p=(1/V)(\partial V/\partial T)_p$ was likewise determined at several different pressures. The entropy of compression at any pressure p could than be found from the relation

$$S_p-S_{\text{sat}}=-\int_{\text{svp}}^{p}V\alpha_p dp, \quad (2)$$

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[1] D. M. Lee and H. A. Fairbank, Phys. Rev. **116**, 1359 (1959).