

Theory of the de Haas–van Alphen effect in two-dimensional superconductors

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(Received 12 May 2000)

The experimentally observed damping of magnetic oscillations in superconductors below B_{c2} is qualitatively explained by application of the Lifshitz-Kosevich formula with the superconducting gap playing the role of the self-energy. In two dimensions this formula omits a leading order term proportional to oscillations of the self-energy. We apply a recently proposed formalism to derive the magnetization oscillation amplitude of two-dimensional superconductors in the (mixed) superconducting state. We find a significant correction to the LK formula, which leads to a sign reversal of the oscillations below B_{c2} .

I. INTRODUCTION

Quantum oscillations of the magnetization [de Haas–van Alphen (dHvA) oscillations] have provided a wealth of information about Fermi surface structure of many materials for more than three decades.¹ This achievement makes use of the quantization condition such that the frequency of oscillations (which are periodic in the inverse magnetic field) is proportional to an extremal area of the Fermi surface. In addition to the frequency spectrum, there is also useful and important information contained in the *amplitude* of oscillations, which depends on interactions in the system.

The first observation of magnetic oscillations in the superconducting state was reported in 1976 by Graebner and Robbins² for the vortex state of NbSe₂. Since then a wide range of superconducting materials has been studied, including V₃Si,^{3,4} NbSe₂,^{5,6} CeRu₂,⁷ YNi₂B₂C,⁸ and Nb₃Sn (Ref. 9) and the organic superconductor κ -(BEDT-TTF)₂Cu(NCS)₂.¹⁰ One goal of all such experiments is to achieve an explicit measurement of the shape of the Fermi surface. A noteworthy example is κ -(BEDT-TTF)₂Cu(NCS)₂, which was shown to be nearly two dimensional.¹¹

The fact that dHvA oscillations persist into the vortex state is a matter that requires careful consideration. Near B_{c2} the cyclotron radius encloses many vortex lines, therefore it is appropriate to average the field strength across the sample. Estimates of the effect of the field inhomogeneity across the flux lattice indicate that it causes a negligible reduction of the oscillation amplitude.¹² All measurements concur that there is no shift of the dHvA frequency at the transition between the superconducting and normal states.

The conventional Lifshitz-Kosevich (LK) formalism¹³ for describing magnetic oscillations in *three dimensions* gives the amplitude of the k th harmonic as

$$A \sim \frac{T \exp(-1/\omega_c \tau)}{\sinh X}, \quad (1)$$

where T is the temperature, $X = 2\pi^2 kT/\omega_c^*$, $\omega_c = eB/m$ is the cyclotron frequency, B is the applied magnetic field, and m is the band mass. The scattering time τ incorporates effects such as disorder. The effective mass m^* which appears in ω_c^* may be determined from the self-energy $\Sigma(x)$, $m^*/m = [1 - \partial \Sigma(x)/\partial x]^{-1}$, and the general form of the LK formula is

$$A \sim \exp(-1/\omega_c \tau) \frac{1}{\beta} \sum_{\omega_l} \exp\left(\frac{-2\pi k}{\omega_c} [\omega_l - \xi(i\omega_l)]\right), \quad (2)$$

where $\xi(i\omega_l)$ is the analytic extension of the self-energy to the imaginary axis. The inverse temperature is $\beta = 1/T$ and $i\omega_l = i(\pi/\beta)(2l+1)$ are Matsubara frequencies. This formula is based on an approximation given by Luttinger¹⁴ which neglects oscillations in the self-energy.

Treating the gap as a self-energy that appears with the onset of the superconducting state, Maki,¹⁵ Stephen,¹⁶ and Springford and Wasserman¹⁷ predicted a drastic reduction of dHvA oscillations upon entering the superconducting (vortex) state from the normal state. Such a reduction has indeed been observed and all recent experiments have interpreted their data in terms of an additional damping factor arising from the gap¹²

$$\xi = -\frac{\Delta^2}{2} \sqrt{\frac{\pi}{\mu \omega_c}}. \quad (3)$$

The strictly two-dimensional case has been studied by Maniv *et al.*¹⁸ and by Bruun *et al.*¹⁹ Both groups considered the expansion of the thermodynamic potential beyond quadratic order in Δ . In this paper we follow the approach of Maki and Stephen; however, Eqs. (1) and (2) are not a complete description of magnetization oscillations in 2D, since oscillations of the self-energy give rise to important corrections.²⁰ We calculate the magnetization oscillations including contributions coming from oscillations of the self-energy and find a significant contribution that is 180° out of phase, leading to a sign reversal of the oscillations below B_{c2} .

II. MAGNETIZATION OSCILLATIONS

The magnetization is derived from the thermodynamic potential, $M = -\partial \Omega / \partial B$. In Ref. 20 it was argued that a suitable approximation to Ω for an interacting system is

$$\Omega = -\frac{1}{\beta} \text{Tr}[\log G^{-1}], \quad (4)$$

where G contains the self-consistent self-energy. This is an approximation which neglects the contribution of crossed

graphs. For a two-dimensional system in a magnetic field the trace is a sum over Landau levels

$$\Omega = -\frac{1}{\beta} \sum_{\omega_m, n} \log[i\omega_m - (n+1/2)\omega_c - \Sigma(i\omega_m)], \quad (5)$$

which is converted to an integral using the Poisson sum formula

$$\Omega = -\frac{1}{\beta} \sum_{\omega_n} \int_{-\mu}^{\infty} \frac{d\epsilon}{\omega_c} \log[i\omega_n - \epsilon - \Sigma(i\omega_n)] \times \left[1 + 2 \sum_{k=1}^{\infty} (-1)^k \cos \frac{2\pi k(\epsilon + \mu)}{\omega_c} \right]. \quad (6)$$

According to Ref. 20, the important contributions to the magnetization oscillations are

$$M_{osc} = M_1 + M_2 \quad (7)$$

$$M_1 = -\frac{4\pi\mu}{m\omega_c^2} \sum_{k=1}^{\infty} (-1)^k \frac{1}{\beta} \sum_{\omega_l > 0} \exp\left(\frac{-2\pi k}{\omega_c} [\omega_l - \xi(i\omega_l)]\right) \times \sin\left(\frac{2\pi k\mu}{\omega_c}\right) \quad (8)$$

$$M_2 = -\frac{2\pi}{\omega_c\beta} \sum_{\omega_l > 0} \frac{\partial \xi(i\omega_l)}{\partial B} \quad (9)$$

where $\xi(i\omega_m) = \text{Im} \Sigma(i\omega_m)$. M_1 is derived from the cosine term inside the square brackets and is just the LK formula given above Eq. (2). M_2 comes from the first term inside the square brackets and is the contribution originating from oscillations in the self-energy which was first introduced in Ref. 20. Generally M_1 leads M_2 by a factor of $(\omega_c/\mu)^{(d-2)/2}$, where d is the dimension; in two dimensions these two terms are formally of the same order. This result is valid for *any* interacting system in two dimensions. In the case of superconductors, Maki and Stephen justified a simple substitution of the expression (3) for the self-energy. We begin the next section by reviewing their arguments.

III. SUPERCONDUCTOR IN A MAGNETIC FIELD

The properties of a superconductor in a magnetic field are governed by the Gorkov equations²¹

$$\left(i\omega_n + \frac{1}{2m} [\nabla_r - ieA(r)]^2 + \mu \right) G(i\omega_n, r, r') + \Delta(r) F^\dagger(i\omega_n, r, r') = \delta(r - r'), \quad (10)$$

$$\left(-i\omega_n + \frac{1}{2m} [\nabla_r + ieA(r)]^2 + \mu \right) F^\dagger(i\omega_n, r, r') - \Delta^*(r) G(i\omega_n, r, r') = 0. \quad (11)$$

$G(i\omega_n, r, r')$ and $F(i\omega_n, r, r')$ are the ordinary and anomalous Green's functions, respectively, $\Delta(r) = (\lambda/\beta) \Sigma_{\omega_n} F(i\omega_n, r, r)$ is the gap function and λ is the coupling strength. The solutions to these equations may be written in integral form

$$G(i\omega_n, r, r') = G^0(i\omega_n, r, r') - \int dr'' G^0(i\omega_n, r, r'') \times \Delta(r'') F^\dagger(i\omega_n, r'', r'), \quad (12)$$

$$F^\dagger(i\omega_n, r, r') = \int dr'' G^0(-i\omega_n, r'', r) \times \Delta^*(r'') G(i\omega_n, r'', r'). \quad (13)$$

The bare Green's function $G^0(i\omega_n, r, r')$ is expressed in terms of the solutions for a single particle in a magnetic field; in 2D this is

$$G^0(i\omega_n, r, r') = \sum_{n, q} \frac{\phi_{n, q}(r) \phi_{n, q}^*(r')}{i\omega_n - (n+1/2)\omega_c}, \quad (14)$$

$$\phi_{n, q}(x, y) = \left(\frac{1}{Ll2^n n! \sqrt{\pi}} \right)^{1/2} e^{iqy - (x-ql)^2/2l^2} H_n\left(\frac{x-ql}{l}\right), \quad (15)$$

where $l = 1/\sqrt{eB}$ is the magnetic length and H_n is a Hermite polynomial. Substituting Eq. (13) into Eq. (12) we find

$$G(i\omega_n, r, r') = G^0(i\omega_n, r, r') - \int dr_1 dr_2 G_0(i\omega_n, r, r_1) \Delta(r_1) \times G_0(-i\omega_n, r_2, r_1) \Delta^*(r_2) G(i\omega_n, r_2, r'). \quad (16)$$

In Eq. (16) we see that $\Delta(r_1)\Delta(r_2)$ serves as an effective potential. Stephen¹⁶ argued that the potential may be obtained by averaging over vortex lines.

$$V(r_1 - r_2) = \langle e^{i\phi(r_1, r_2)} \Delta(r_1) \Delta^*(r_2) \rangle, \quad (17)$$

where $\phi(r_1, r_2) = (x_2 + x_1)(y_2 - y_1)/l^2$ in the Landau gauge, and the gap function is²²

$$\Delta(r) = \sum_n C_n e^{iqny} \exp\left[-\frac{1}{l^2} \left(x - \frac{nql^2}{2}\right)^2\right]. \quad (18)$$

Stephen calculated $V(r)$ using both a square vortex lattice ($C_n = 1$) and a disordered vortex lattice. It is not difficult to show that a triangular vortex lattice ($C_n = C_{n+2}, C_1 = iC_0$) yields the same result. In all of these cases one finds

$$V(r) = \Delta^2 e^{-r^2/2l^2}, \quad (19)$$

where Δ is the magnitude of the gap. The potential $V(r_1 - r_2)$ satisfies the self-consistent equation derived from Eq. (13) by setting $r = r' = r_2$, multiplying both sides by $\Delta(r_1) e^{i\phi(r_1, r_2)}$ and averaging

$$V(r_1 - r_2) = \frac{\lambda}{\beta} \sum_{\omega_n} \int dr V(r - r_1) G(i\omega_n, r, r_2) \times G^0(-i\omega_n, r, r_2) e^{i\phi(r_1, r_2)} e^{i\phi(r, r_1)} \quad (20)$$

(see the Appendix).

The solution for $G(i\omega_n, r)$ is of the form

$$G(i\omega_n, r, r') = \sum_{n, q} \frac{\phi_{n, q}(r) \phi_{n, q}^*(r')}{i\omega_n - (n+1/2)\omega_c - \Sigma(i\omega_n, n)}. \quad (21)$$

One may find Σ by substituting Eqs. (19) and (21) into Eq. (16) and performing the required integrations²³

$$\Sigma(i\omega_n, n) = \Delta^2 \sum_{n'} \frac{I_{nn'}}{i\omega_n + (n' + 1/2)\omega_c}, \quad (22)$$

$$I_{nn'} = \frac{(n+n')!}{n!n'!2^{n+n'+1}}. \quad (23)$$

This result indicates that the self-energy has very large oscillations and is actually singular at the energy of each Landau level. For this reason it is better to improve the calculation by solving for the self-energy self-consistently, by substituting the full Green's function $G(-i\omega_n, r_2, r_1)$ in Eq. (16). Then Σ satisfies

$$\Sigma(i\omega_n, n) = \Delta^2 \sum_{n'} \frac{I_{nn'}}{i\omega_n + (n' + 1/2)\omega_c + \Sigma(-i\omega_n, n')}. \quad (24)$$

Assuming that the largest contributions to the sum over n' come near the pole of Σ one finds for $n' \approx n \approx \nu$ that $I_{nn'} \approx 1/\sqrt{4\pi\nu}$. Here ν is the number of filled Landau levels. Now write $\Sigma = \bar{\Sigma} + \Sigma_{\text{osc}}$ and solve Eq. (24) under the assumption that $\Sigma_{\text{osc}} \ll \bar{\Sigma}$. The left hand side of Eq. (24) can be expanded using the Poisson sum formula

$$\begin{aligned} \bar{\Sigma}(i\omega_n) + \Sigma_{\text{osc}}(i\omega_n) &= \frac{\Delta^2}{\sqrt{4\pi\nu}} \int_{-\mu\omega_c}^{\infty} \frac{d\epsilon}{i\omega_n + \epsilon + \bar{\Sigma}(-i\omega_n)} \\ &\times \left[1 + 2 \sum_{k=1}^{\infty} (-1)^k \cos \frac{2\pi k(\epsilon + \mu)}{\omega_c} \right]. \end{aligned} \quad (25)$$

The second term in the square brackets shows oscillations explicitly in terms of the cosine. $\bar{\Sigma}$ is found by omitting all of the oscillatory parts and taking both limits of the integral to infinity,

$$\bar{\Sigma}(i\omega_n) = -\frac{i\pi\Delta^2}{\sqrt{4\pi\nu}\omega_c} \text{sgn}(\omega_n). \quad (26)$$

This result was obtained by Stephen.¹⁶ The oscillatory part is obtained by splitting the cosine and expressing the ϵ dependent parts as exponentials, and then integrating over the top/bottom half planes as dictated by the signs of the exponentials

$$\begin{aligned} \Sigma_{\text{osc}}(i\omega_n) &= \frac{i2\pi\Delta^2}{\sqrt{4\pi\nu}\omega_c} \sum_{k=1}^{\infty} (-1)^k \left(-\text{sgn}(\omega_n) \cos \frac{2\pi k\mu}{\omega_c} \right. \\ &\quad \left. + i \sin \frac{2\pi k\mu}{\omega_c} \right) \exp\left(-\frac{2\pi k}{\omega_c} \left| \omega_n - \bar{\Sigma}(i\omega_n) \right| \right). \end{aligned} \quad (27)$$

Finally we substitute the results (26) and (27) into the equations for the magnetization (8) and (9), and calculate the sum over ω_l . The first term is the Maki-Stephen result

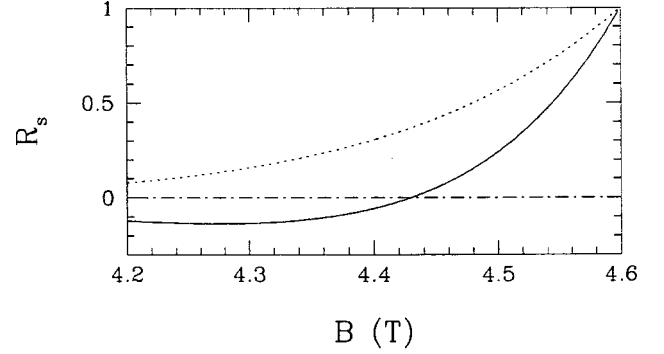


FIG. 1. The amplitude of the first harmonic of magnetization oscillations for κ -(BEDT-TTF)₂Cu(NSC)₂ below B_{c2} using the parameters given in the text. The solid line is $M_1 + M_2$ and the dotted line is the Maki-Stephen result (M_1 only).

$$\begin{aligned} M_1 &= -\frac{2\pi}{m} \frac{\mu}{\omega_c^2} \frac{1}{\beta} \sum_{k=1}^{\infty} (-1)^k \\ &\times \frac{\exp(-2\pi^2 k \Delta^2 / \omega_c^2 \sqrt{4\pi\nu})}{\sinh(2\pi^2 k T / \omega_c)} \sin \frac{2\pi k \mu}{\omega_c}. \end{aligned} \quad (28)$$

The second term is

$$\begin{aligned} M_2 &= \frac{4\pi^3}{m\sqrt{4\pi\nu}} \frac{\Delta^2}{\omega_c^2} \frac{\mu}{\omega_c^2} \frac{1}{\beta} \sum_{k=1}^{\infty} (-1)^k k \\ &\times \frac{\exp(-2\pi^2 k \Delta^2 / \omega_c^2 \sqrt{4\pi\nu})}{\sinh(2\pi^2 k T / \omega_c)} \sin \frac{2\pi k \mu}{\omega_c}. \end{aligned} \quad (29)$$

Equation (29) is the main result of this paper. The most important feature of M_2 is that the coefficient is of the same order in μ/ω_c as in M_1 , a result which is unique to two dimensions.²⁰ The remaining coefficients may be considered to be the coupling constant of the self-energy, and in many systems this constant is small, providing a justification for the LK formula even in 2D. However here the effective coupling may be rather large; using estimates given in Ref. 10 for κ -(BEDT-TTF)₂Cu(NSC)₂ in the regime below B_{c2} we have $\Delta \approx 1$ meV, $\omega_c \approx 0.1$ meV and $\nu = F/B \approx 100$ (where F is the dHvA frequency), resulting in a coefficient for M_2 that is the same order of magnitude as that of M_1 . However, it is difficult to make a detailed comparison between this result and experiments, since the quantities B_{c2} and $\Delta(0)$ which appear in the expression for the gap, $\Delta(B) = \Delta(0)\sqrt{1 - B/B_{c2}}$ are not known exactly.

The amplitude of M_{SC}/M_N (which is called R_s in Ref. 12) is plotted in Fig. 1, using $m = 3.5m_e$, $F = 600$ T, $\Delta(0) = 1.6$ meV, and $B_{c2} = 4.6$ T. The amplitude rapidly becomes negligible below B_{c2} and changes sign within a few periods of oscillation. The ratio M_{SC}/M_N contains a factor which equals one at B_{c2} of the form

$$1 - \frac{2\pi^2 k \Delta^2}{\sqrt{4\pi\nu} \omega_c^2}. \quad (30)$$

The vanishing of this factor marks a 180° change of phase of the oscillations. Reference 18 found a similar effect in a slightly different form. In contrast, the numerical work of

Norman and MacDonald²⁴ found that no such phase change occurs if Δ is determined self-consistently in a full off-diagonal calculation. In the Appendix we have shown that Eq. (27) satisfies the self-consistent equation for Δ , therefore there are no corrections to Eq. (30), at least to within the diagonal approximation.

In summary, we present straightforward, yet hitherto neglected, extension of Luttinger's formalism for interacting systems in two dimensions. We find that oscillations in the self-energy yield an important contribution to the amplitude of magnetization oscillations in the vortex state of two-dimensional superconductors which leads to a change in sign of the oscillations below B_{c2} .

ACKNOWLEDGMENTS

The author acknowledges Philip Stamp for previous collaboration, and the Weizmann Institute of Science where this work was begun. This work was supported by NSERC of Canada.

APPENDIX

In this appendix we show that oscillations which appear in the self-consistent equation for the potential $V(r_1 - r_2)$ are fully accounted for by the oscillations in the self-energy, provided that the gap function satisfies a gap equation. We begin by noting that the usual BCS gap equation is obtained from the self-consistent equation for $V(r_1 - r_2)$ (20) using the simplest form¹⁶ of Σ [Eq. (22)]. However, the main part of this article prescribes a more complicated calculation which uses two full Green's functions in Eq. (20) and the self-consistent self-energy (24). In Eq. (20) we expand the Green's functions in q_1, q_2, n_1, n_2 and integrate over r, q_1 and q_2 to get

$$1 = \frac{\lambda}{l^2 \beta} \sum_{\omega_n, n_1, n_2} G(i\omega_n, n_1) G(-i\omega_n, n_2) I_{n_1 n_2}. \quad (\text{A1})$$

One of the sums over Landau levels is dropped using the diagonal approximation, $I_{n_1 n_2} \approx \delta_{n_1 n_2} \sqrt{4\pi\nu}$ and then the remaining sum is replaced by an integral using the Poisson sum formula

$$1 = -\frac{1}{l^2 \sqrt{4\pi\nu}} \frac{\lambda}{\beta} \sum_{i\omega_n} \int_{-\mu\omega_c}^{\infty} \frac{d\epsilon}{\omega_n - \epsilon - \Sigma(i\omega_n)} \times \frac{1}{i\omega_n + \epsilon - \bar{\Sigma}(i\omega_n)} \left[1 + 2 \sum_{k=1}^{\infty} (-1)^k \cos \frac{2\pi k(\epsilon + \mu)}{\omega_c} \right]. \quad (\text{A2})$$

Note that $\Sigma(-i\omega_n) = -\Sigma(i\omega_n)$. The self-energy is split into oscillatory and nonoscillatory parts $\Sigma = \bar{\Sigma} + \Sigma_{\text{osc}}$, where $\bar{\Sigma}$ satisfies

$$1 = -\frac{1}{l^2 \sqrt{4\pi\nu}} \frac{\lambda}{\beta} \sum_{\omega_n} \int_{-\mu\omega_c}^{\infty} \frac{d\epsilon}{i\omega_n - \epsilon - \bar{\Sigma}(i\omega_n)} \times \frac{1}{i\omega_n + \epsilon - \bar{\Sigma}(i\omega_n)}. \quad (\text{A3})$$

Expressing $\bar{\Sigma}$ in terms of Δ^2 with Eq. (26) leads to a cutoff dependent solution for Δ . Then, the first term inside the square brackets of Eq. (A2) may be integrated and then expanded as

$$-\frac{1}{l^2 \sqrt{4\pi\nu}} \frac{\lambda}{\beta} \sum_{\omega_n} \int_{-\mu\omega_c}^{\infty} \frac{d\epsilon}{\omega_n - \epsilon - \bar{\Sigma}(i\omega_n)} \frac{1}{i\omega_n + \epsilon - \bar{\Sigma}(i\omega_n)} = \frac{1}{l^2 \sqrt{4\pi\nu}} \frac{\lambda}{\beta} \sum_{\omega_n} \frac{i\pi}{\omega_c} \frac{\text{sgn}(\omega_n)}{i\omega_n - \bar{\Sigma}(i\omega_n) - \Sigma_{\text{osc}}(i\omega_n)} \approx 1 + \frac{1}{l^2 \sqrt{4\pi\nu}} \frac{\lambda}{\beta} \sum_{\omega_n} \frac{i\pi}{\omega_c} \frac{\Sigma_{\text{osc}}(i\omega_n) \text{sgn}(\omega_n)}{[i\omega_n - \bar{\Sigma}(i\omega_n)]^2}. \quad (\text{A4})$$

Substituting Eq. (A4) into Eq. (A2) we find that

$$i\pi \sum_{\omega_n} \frac{\Sigma_{\text{osc}}(i\omega_n) \text{sgn}(\omega_n)}{[i\omega_n - \bar{\Sigma}(i\omega_n)]^2} = \sum_{\omega_n} \int_{-\mu\omega_c}^{\infty} \frac{d\epsilon}{\omega_n - \epsilon - \bar{\Sigma}(i\omega_n)} \frac{1}{i\omega_n + \epsilon - \bar{\Sigma}(i\omega_n)} \times 2 \sum_{k=1}^{\infty} (-1)^k \cos \frac{2\pi k(\epsilon + \mu)}{\omega_c}. \quad (\text{A5})$$

Extending the limits of the integral to $\pm\infty$ the right hand side of Eq. (A5) is

$$-i2\pi \sum_{\omega_n} \frac{\text{sgn}(\omega_n)}{i\omega_n - \bar{\Sigma}(i\omega_n)} \sum_{k=1}^{\infty} (-1)^k \cos \frac{2\pi k\mu}{\omega_c} \times \exp\left(-\frac{2\pi k}{\omega_c} \left| \omega_n - \bar{\Sigma}(i\omega_n) \right| \right).$$

The left hand side of Eq. (A5) is found using Eqs. (27) and (26),

$$i2\pi \sum_{\omega_n} \frac{|\bar{\Sigma}(\omega_n)|}{(i\omega_n - \bar{\Sigma}(i\omega_n))^2} \sum_{k=1}^{\infty} (-1)^k \cos \frac{2\pi k\mu}{\omega_c} \times \exp\left(-\frac{2\pi k}{\omega_c} \left| \omega_n - \bar{\Sigma}(i\omega_n) \right| \right).$$

Equality of both sides of Eq. (A5) is obtained when $\bar{\Sigma} \gg \omega_n$, or $\Delta^2/\omega_c \gg T$. This result shows that there are no additional oscillations in the gap; within the approximations used all oscillatory effects are accounted for within $\bar{\Sigma}$.

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