Supplemental materials to "Magnetization of topological line-node semimetals"

G. P. Mikitik and Yu. V. Sharlai
B. Verkin Institute for Low Temperature Physics & Engineering, Ukrainian Academy of Sciences, Kharkov 61103, Ukraine

DERIVATION OF FORMULAS FOR Ω POTENTIAL AND MAGNETIZATION

We start with the common expression for the Ω-potential per the unit volume (see, e.g., [1, 2]):

$$\Omega_H = -\frac{2T}{(2\pi\hbar)^2}\frac{eH}{c}\sum_{c,v}\sum_{l=0}^{\infty}{}' \int_0^L dp_3 \cos\theta \ln\left(1+\exp\frac{\zeta-\varepsilon^l_{c,v}(p_3)}{T}\right), \tag{1}$$

where ζ is the chemical potential, T is the temperature, the electron energy in the magnetic field, $\varepsilon^l_{c,v}(p_3)$, is given by the equations,

$$\varepsilon^l_{c,v}(p_3) = \varepsilon_d(p_3) \pm \left(\frac{e\hbar\alpha H|\cos\theta|}{c}l\right)^{1/2}, \tag{2}$$

$$\alpha = \alpha(p_3) = 2(b_{11}b_{22})^{1/2}(1-\tilde{a}_\perp^2)^{3/2}, \tag{3}$$

the prime near the sum means that the term corresponding to $l = 0$ is taken with the additional factor 1/2, the integration is carried out over the length L of the band-contact line in the Brillouin zone, $\theta = \theta(p_3)$ is angle between the magnetic field $\mathbf{H}$ and the tangent to the band-contact line at the point p_3. In Eq. (2) and formulas below, the signs "+" and "−" correspond to the conduction "c" and valence "v" bands, respectively. We have also assumed the two-fold degeneracy of these bands in spin. With Eq. (2), it is clear that Ω_H is expressed in terms of the combination $H_3 = H\cos\theta$. We calculate only the part of the Ω_H that depends on the magnetic field,

$$\Omega(\zeta, H) = \Omega_H - \Omega_0\,, \tag{4}$$

where $\Omega_0 = \lim_{H\to 0}\Omega_H$ is the Ω-potential at zero magnetic field. At $T = 0$ we obtain from Eq. (1):

$$\Omega(\zeta,H) = -\frac{e^{3/2}}{2\pi^2\hbar^{3/2}c^{3/2}}\sum_{c,v}\int_0^L dp_3\sqrt{\alpha(p_3)}H_3\sum_{l=0}^{\infty}{}'\left(w\pm\sqrt{H_3 l}\right)\sigma\left(w\pm\sqrt{H_3 l}\right)$$
$$+\frac{e^{3/2}}{2\pi^2\hbar^{3/2}c^{3/2}}\sum_{c,v}\int_0^L dp_3\sqrt{\alpha(p_3)}\int_0^\infty dx\left(w\pm\sqrt{x}\right)\sigma\left(w\pm\sqrt{x}\right), \tag{5}$$

where $\sigma(x) = 1$ if $x > 0$, and $\sigma(x) = 0$ if $x < 0$, and

$$w \equiv \frac{[\zeta-\varepsilon_d(p_3)]\sqrt{c}}{\sqrt{e\hbar\alpha(p_3)}}. \tag{6}$$

Formula (5) can be rearranged as follows:

$$\Omega(\zeta,H) = -\frac{e^{3/2}}{2\pi^2\hbar^{3/2}c^{3/2}}\sum_{c,v}\int_0^L dp_3\sqrt{\alpha(p_3)}H_3\Big[\frac{1}{2}w\sigma(w) - \int_0^{1/2}dl'(w\pm\sqrt{H_3 l'}))\sigma(w\pm\sqrt{H_3 l'})$$
$$+\sum_{l=1}^{\infty}\left\{(w\pm\sqrt{H_3 l})\sigma(w\pm\sqrt{H_3 l}) - \int_{l-1/2}^{l+1/2}dl'(w\pm\sqrt{H_3 l'})\sigma(w\pm\sqrt{H_3 l'})\right\}\Big], \tag{7}$$

where we have made the formal substitution $x = H_3 l'$. Using the identity $\sigma(x)+\sigma(-x)\equiv 1$, one can show that

$$\sum_{c,v}(w\pm\sqrt{H_3 l})\sigma(w\pm\sqrt{H_3 l}) = 2w + \sum_{c,v}(-w\pm\sqrt{H_3 l})\sigma(-w\pm\sqrt{H_3 l}), \quad w\sigma(w) = w - w\sigma(-w). \tag{8}$$

Hence, $\Omega(\zeta,H)$ in Eq. (7) does not depend on a sign of the w, and we can replace w by $|w|$ in Eq. (7). Using also the fact that $\sigma(|w|+\sqrt{H_3 l})=1$, we arrive at

$$\Omega(\zeta,H)=-\frac{e^{3/2}}{2\pi^2\hbar^{3/2}c^{3/2}}\int_0^L dp_3\sqrt{\alpha(p_3)}H_3\Big[|w|-\int_0^{1/2}dl'(|w|+\sqrt{H_3 l'}))-\int_0^{1/2}dl'(|w|-\sqrt{H_3 l'}))\sigma(|w|-\sqrt{H_3 l'})$$
$$+\sum_{l=1}^{\infty}\left\{(|w|+\sqrt{H_3 l})-\int_{l-1/2}^{l+1/2}dl'(|w|+\sqrt{H_3 l'})\right\}$$
$$+\sum_{l=1}^{\infty}\left\{(|w|-\sqrt{H_3 l})\sigma(|w|-\sqrt{H_3 l})-\int_{l-1/2}^{l+1/2}dl'(|w|-\sqrt{H_3 l'})\sigma(|w|-\sqrt{H_3 l'})\right\}\Big] \tag{9}$$

Note that the last sum in Eq. (9) is, in fact, finite due to the factor σ. Combining all the integrals containing $\sigma(|w|-\sqrt{H_3 l'})$, we obtain

$$\int_0^{\infty}dl'(|w|-\sqrt{H_3 l'})\sigma(|w|-\sqrt{H_3 l'})=\int_0^{w^2/H_3}dl'(|w|-\sqrt{H_3 l'})=\frac{1}{3}\frac{|w|^3}{H_3}, \tag{10}$$

and

$$\Omega(\zeta,H)=-\frac{e^{3/2}}{2\pi^2\hbar^{3/2}c^{3/2}}\int_0^L dp_3\sqrt{\alpha(p_3)}H_3\Big[\frac{1}{2}|w|-\sqrt{H_3}\frac{1}{3\sqrt{2}}$$
$$+\sqrt{H_3}\sum_{l=1}^{\infty}\left\{l^{1/2}-\frac{2}{3}((l+\frac{1}{2})^{3/2}-(l-\frac{1}{2})^{3/2})\right\}$$
$$+\sum_{l=1}^{[u]}\left\{(|w|-\sqrt{H_3 l})\right\}-\frac{|w|^3}{3H_3}\Big], \tag{11}$$

where $[u]$ means the integer part of u,

$$u(p_3)\equiv\frac{w^2}{H_3}=\frac{[\zeta-\varepsilon_d(p_3)]^2c}{e\hbar\alpha(p_3)H|\cos\theta|}=\frac{cS(p_3)}{2\pi e\hbar H}, \tag{12}$$

and $S(p_3)$ is the area of the cross section of the Fermi surface by the plane perpendicular to the magnetic field and passing through the point with the coordinate p_3. Thus, equation (11) reduces to the formula:

$$\Omega(\zeta,H)=-\frac{e^{3/2}}{2\pi^2\hbar^{3/2}c^{3/2}}\int_0^L dp_3\sqrt{\alpha(p_3)}\Big\{H_3^{3/2}\Big[\sum_{l=1}^{\infty}\left(l^{1/2}-\frac{2}{3}\left[\left(l+\frac{1}{2}\right)^{3/2}-\left(l-\frac{1}{2}\right)^{3/2}\right]\right)-\frac{2}{3}\left(\frac{1}{2}\right)^{3/2}\Big]$$
$$+H_3|w|\left([u]+\frac{1}{2}\right)-H_3^{3/2}\sum_{l=1}^{[u]}l^{1/2}-\frac{1}{3}|w|^3\Big\}. \tag{13}$$

Using the relation

$$\zeta(-\frac{1}{2},l)-l^{1/2}=\zeta(-\frac{1}{2},l+1) \tag{14}$$

for the Hurwitz zeta function $\zeta(-1/2,x)$, and the asymptotic expansion of this function at $x\gg 1$ [3]:

$$\zeta(-1/2,x)=-\frac{2}{3}x^{3/2}+\frac{1}{2}x^{1/2}-\frac{1}{24x^{1/2}}+O(\frac{1}{x^{3/2}}), \tag{15}$$

one can calculate the sums in Eq. (13),

$$\sum_{l=1}^{\infty}\left(l^{1/2}-\frac{2}{3}\left[\left(l+\frac{1}{2}\right)^{3/2}-\left(l-\frac{1}{2}\right)^{3/2}\right]\right)-\frac{2}{3}\left(\frac{1}{2}\right)^{3/2}-\sum_{l=1}^{[u]}l^{1/2}=$$
$$\lim_{M\to\infty}\Big[\sum_{l=1}^{M}\left(l^{1/2}-\frac{2}{3}\left[\left(l+\frac{1}{2}\right)^{3/2}-\left(l-\frac{1}{2}\right)^{3/2}\right]\right)-\frac{2}{3}\left(\frac{1}{2}\right)^{3/2}-\sum_{l=1}^{[u]}l^{1/2}\Big]=$$
$$\lim_{M\to\infty}\Big[\sum_{l=[u]+1}^{M}l^{1/2}-\frac{2}{3}(M+\frac{1}{2})^{3/2}\Big]=$$
$$\lim_{M\to\infty}\Big[\sum_{l=[u]+1}^{M}[\zeta(-\frac{1}{2},l)-\zeta(-\frac{1}{2},l+1)]-\frac{2}{3}(M+\frac{1}{2})^{3/2}\Big]=$$
$$\lim_{M\to\infty}\Big[\zeta(-\frac{1}{2},[u]+1)-\zeta(-\frac{1}{2},M+1)-\frac{2}{3}(M+\frac{1}{2})^{3/2}\Big]=$$
$$\lim_{M\to\infty}\Big[\zeta(-\frac{1}{2},[u]+1)+\frac{2}{3}(M+1)^{3/2}-\frac{1}{2}(M+1)^{1/2}-\frac{2}{3}(M+\frac{1}{2})^{3/2}\Big]=\zeta(-\frac{1}{2},[u]+1). \quad (16)$$

Eventually, we obtain the following expressions for the Ω potential and the magnetization at $T=0$:

$$\Omega(\zeta,H)=-\frac{e^{3/2}H^{3/2}}{2\pi^2\hbar^{3/2}c^{3/2}}\int_0^L dp_3|\cos\theta|^{3/2}\sqrt{\alpha(p_3)}K_1(u), \quad (17)$$
$$\mathbf{M}(\zeta,H)=\frac{e^{3/2}H^{1/2}}{2\pi^2\hbar^{3/2}c^{3/2}}\int_0^L dp_3|\cos\theta|^{1/2}\nu\sqrt{\alpha(p_3)}K(u)\mathbf{t}, \quad (18)$$

where $\mathbf{t}=\mathbf{t}(p_3)$ is the unit vector along the tangent to the band-contact line at a point p_3; $\nu=\nu(p_3)$ is a sign of $\cos\theta$;

$$K_1(u)=\zeta(-\frac{1}{2},[u]+1)+\sqrt{u}([u]+\frac{1}{2})-\frac{1}{3}u^{3/2}, \quad (19)$$
$$K(u)=\frac{3}{2}\zeta(-\frac{1}{2},[u]+1)+\sqrt{u}([u]+\frac{1}{2}), \quad (20)$$

For nonzero temperatures, the Ω potential and the magnetization $M_i(\zeta,H,T)$ can be calculated with the relationships [2]:

$$\Omega(\zeta,H,T)=-\int_{-\infty}^{\infty}d\varepsilon\Omega(\varepsilon,H,0)f'(\varepsilon), \quad (21)$$
$$M_i(\zeta,H,T)=-\int_{-\infty}^{\infty}d\varepsilon M_i(\varepsilon,H,0)f'(\varepsilon), \quad (22)$$

where $f'(\varepsilon)$ is the derivative of the Fermi function,

$$f'(\varepsilon)=-\left[4T\cosh^2\left(\frac{\varepsilon-\zeta}{2T}\right)\right]^{-1}. \quad (23)$$

WEAK MAGNETIC FIELDS

Consider the expression for the Ω potential in the limiting case of the weak magnetic field, $H\ll H_T$. Specifically, we shall assume that

$$u_T=\frac{T^2c}{e\hbar\alpha(p_3)H|\cos\theta|}\gg 1. \quad (24)$$

Inserting formula (17) into Eq. (21), interchanging the order of the integrations, and replacing ε by the variable $\sqrt{u}$ defined by the formula,

$$\varepsilon=\varepsilon_d(p_3)\pm\frac{(e\hbar\alpha(p_3)H|\cos\theta|)^{1/2}}{c^{1/2}}\sqrt{u},$$

we arrive at

$$\Omega(\zeta,H,T)=\frac{e^2H^2}{\pi^2\hbar c^2}\int_0^L dp_3\cos^2\theta\alpha(p_3)f'(\varepsilon_d(p_3))I, \tag{25}$$

where

$$I=\int_0^\infty d(\sqrt{u})K_1(u). \tag{26}$$

In deriving (25), we have replaced ε by $\varepsilon_d(p_3)$ in the argument of the function $f'(\varepsilon)$. This replacement is based on the assumption that one can choose a constant u_0 so that $1\ll u_0\ll u_T$ (and hence $|\varepsilon(u_0)-\varepsilon_d(p_3)|\ll T$) and at the same time $|I-I(u_0)|\ll|I|$, where

$$I(u_0)\equiv\int_0^{\sqrt{u_0}} d(\sqrt{u})K_1(u). \tag{27}$$

To justify this assumption and to find I, let us calculate $I(u_0)$ which can be rewritten as follows:

$$I(u_0)=\sum_{n=0}^{[u_0]-1}\int_{\sqrt{n}}^{\sqrt{n+1}} d(\sqrt{u})K_1(u)+\int_{\sqrt{[u_0]}}^{\sqrt{u_0}} d(\sqrt{u})K_1(u), \tag{28}$$

where $[u_0]$ is the integer part of u_0. With Eq. (19), we have

$$\begin{aligned}\int_{\sqrt{n}}^{\sqrt{n+1}} d(\sqrt{u})K_1(u) &= \zeta(-\frac{1}{2},n+1)(\sqrt{n+1}-\sqrt{n})\\ &+ (n+\frac{1}{2})\frac{1}{2}-\frac{1}{12}[(n+1)^2-n^2]=\frac{2n+1}{6}\\ &+ \zeta(-\frac{1}{2},n+1)(\sqrt{n+1}-\sqrt{n}).\end{aligned} \tag{29}$$

Taking into account the relation (14), we obtain

$$\begin{aligned}&\sum_{n=0}^{[u_0]-1}\zeta(-\frac{1}{2},n+1)(\sqrt{n+1}-\sqrt{n})=\sum_{n=1}^{[u_0]}\zeta(-\frac{1}{2},n)\sqrt{n}\\ &-\sum_{n=1}^{[u_0]-1}\zeta(-\frac{1}{2},n+1)\sqrt{n}=\zeta(-\frac{1}{2},[u_0])\sqrt{[u_0]}\\ &+\sum_{n=1}^{[u_0]-1}[\zeta(-\frac{1}{2},n)-\zeta(-\frac{1}{2},n+1)]\sqrt{n}=\zeta(-\frac{1}{2},[u_0])\sqrt{[u_0]}\\ &+\frac{[u_0]([u_0]-1)}{2},\end{aligned} \tag{30}$$

and

$$\begin{aligned}\sum_{n=0}^{[u_0]-1}\int_{\sqrt{n}}^{\sqrt{n+1}} d(\sqrt{u})K_1(u) &= \zeta(-\frac{1}{2},[u_0])\sqrt{[u_0]}\\ &+\frac{2[u_0]^2}{3}-\frac{[u_0]}{2}.\end{aligned} \tag{31}$$

Using the asymptotic expansion (15) for $\zeta(-1/2,x)$ at $x\gg1$, one can estimate the sum (31) and the last term in the right hand side of Eq. (28),

$$\sum_{n=0}^{[u_0]-1}\int_{\sqrt{n}}^{\sqrt{n+1}} d(\sqrt{u})K_1(u) = -\frac{1}{24}+O(\frac{1}{[u_0]}), \tag{32}$$

$$\int_{\sqrt{[u_0]}}^{\sqrt{u_0}} d(\sqrt{u})K_1(u) \approx -\frac{\{u\}}{48[u_0]}(1-3\{u\}+2\{u\}^2)=O(\frac{1}{[u_0]}),$$

where $\{u\} \equiv u_0 - [u_0] < 1$. Inserting formulas (32) into Eq. (28), we eventually find that

$$I(u_0) = -\frac{1}{24} + O(\frac{1}{[u_0]}),$$

$I = -1/24$, and hence

$$\Omega(\zeta, H, T) = -\frac{e^2 H^2}{24\pi^2 \hbar c^2} \int_0^L dp_3 \cos^2\theta \alpha(p_3) f'(\varepsilon_d(p_3)), \tag{33}$$

With this Ω potential, we arrive at linear dependence of the magnetization $\mathbf{M} = -\partial\Omega/\partial\mathbf{H}$ on the magnetic field,

$$\mathbf{M}(\zeta, H, T) = \frac{e^2 H}{12\pi^2 \hbar c^2} \int_0^L dp_3 (\cos\theta) \alpha(p_3) f'(\varepsilon_d) \mathbf{t}. \tag{34}$$

Finally, it is necessary to emphasize that if we started with Eq. (18) for the magnetization rather than with Eq. (17) for the Ω potential and used the same approach in analyzing the case of weak magnetic fields, we would not obtain the correct expression (34) for the magnetization. This is due to the fact that the integral $\int_0^\infty K(u) d\sqrt{u}$ does not converge (the integral $\int_0^{u_0} K(u) d\sqrt{u}$ oscillates with changing u_0, and the amplitude of these oscillations does not tend to zero at large u_0).

THE DE HAAS - VAN ALPHEN OSCILLATIONS

The quantity u defined by Eq. (12) changes along the nodal line from its minimal value u_{min} to its maximal value u_{max}. These extremal values of u correspond to minimal and maximal areas (in p_3) of Fermi-surface cross sections by planes perpendicular to the magnetic field. Consider Eq. (18) in the case when

$$u_{min},\ u_{max},\ u_{max} - u_{min} \gg 1. \tag{35}$$

Using Eqs. (15) and (20), we obtain for large u:

$$K(u) \approx \frac{1}{2}\sqrt{u}(\{u\} - \frac{1}{2}) = -\frac{\sqrt{u}}{2\pi} \sum_{n=1}^{\infty} \frac{\sin(2\pi n u)}{n}, \tag{36}$$

where $\{u\} = u - [u]$, and $[u]$ is the integer part of u. Thus, the integrand in Eq. (18) highly oscillates about zero, and only the band-contact-line portions located near the points at which u reaches the extremal values give contributions to Eq. (18). Let u reach the extremal value u_{ex} at the point p_3^{ex}, and let us calculate the appropriate contribution to the magnetization. Near p_3^{ex} we can write the following expansion for $u(p_3)$:

$$u(p_3) \approx u_{ex} \pm \frac{1}{2} \left| \frac{\partial^2 S}{\partial p_3^2} \right| \frac{c}{2\pi e \hbar H} (p_3 - p_3^{ex})^2 \equiv u_{ex} \pm B(\delta p_3)^2, \tag{37}$$

where $\delta p_3 \equiv p_3 - p_3^{ex}$, $u_{ex} = u_{min}$ or u_{max}, the upper sign corresponds to u_{min} and the lower sign to u_{max}. Inserting Eqs. (36) and (37) into formula (18), we arrive at

$$\mathbf{M}(\zeta, H) \approx -\frac{e}{4\pi^3 \hbar^2 c} \sum_{n=1}^{\infty} \frac{|\zeta - \varepsilon_d(p_3^{ex})| (\nu \mathbf{t})_{p_3 = p_3^{ex}}}{n} \int dp_3 \big(\sin(2\pi n u_{ex}) \cos[2\pi n B(\delta p_3)^2] \pm \cos(2\pi n u_{ex}) \sin[2\pi n B(\delta p_3)^2] \big). \tag{38}$$

One may set the infinite limits in this integral over p_3. Then, we find

$$\mathbf{M}(\zeta, H) \approx -\left(\frac{e}{\hbar c}\right)^{3/2} \frac{H^{1/2}}{2\sqrt{2}\pi^{5/2}} \left| \frac{\partial^2 S}{\partial p_3^2} \right|^{-1/2} |\zeta - \varepsilon_d(p_3^{ex})| (\nu \mathbf{t})_{p_3 = p_3^{ex}} \sum_{n=1}^{\infty} \frac{1}{n^{3/2}} \sin\left(n \frac{c S_{ex}}{e \hbar H} \pm \frac{\pi}{4} \right), \tag{39}$$

where the expressions for B, Eq. (37), and for u_{ex}, Eq. (12), have been inserted; S_{ex} is the area of the extremal cross section perpendicular to the magnetic field. Formula (39) describes the de Haas - van Alphen oscillations. In particular, we obtain the followin expression for the magnetization component $M_{\parallel}$ parallel to the magnetic field:

$$M_{\parallel}(\zeta, H) \approx -\left(\frac{e}{\hbar c}\right)^{3/2} \frac{H^{1/2}}{2\sqrt{2}\pi^{5/2}} \left| \frac{\partial^2 S}{\partial p_3^2} \right|^{-1/2} |\zeta - \varepsilon_d(p_3^{ex})| \, |\cos[\theta(p_3^{ex})]| \sum_{n=1}^{\infty} \frac{1}{n^{3/2}} \sin\left(n \frac{c S_{ex}}{e \hbar H} \pm \frac{\pi}{4} \right). \tag{40}$$

Compare Eq. (40) with the well-known formula describing the de Haas - van Alphen effect at $T = 0$ [1, 4–6],

$$M_{\parallel}(\zeta, H) \approx -\left(\frac{e}{\hbar c}\right)^{3/2} \frac{H^{1/2} S_{ex}}{2\sqrt{2}\pi^{7/2}|m_*|} \left|\frac{\partial^2 S}{\partial p_z^2}\right|^{-1/2} \sum_{n=1}^{\infty} \frac{1}{n^{3/2}} \sin\!\left(2\pi n\left(\frac{cS_{ex}}{2\pi e\hbar H} - \gamma\right) \pm \frac{\pi}{4}\right), \qquad (41)$$

where the component p_z is along the magnetic field, m_* is the cyclotron mass, the constant γ appears in the semi-classical quantization rule,

$$S(\varepsilon) = \frac{2\pi e\hbar H}{c}(n + \gamma), \qquad (42)$$

and is expressed in term of the Berry phase Φ_B for the appropriate electron orbit [7]:

$$\gamma = \frac{1}{2} - \frac{\Phi_B}{2\pi}. \qquad (43)$$

If the electron orbit surrounds a band-contact line, $\Phi_B = \pi$ and $\gamma = 0$; otherwise $\Phi_B = 0$ and $\gamma = 1/2$ [7]. In Eq. (41), as in Eqs. (18) and (40), we completely neglect the electron spin. In the case a line-node semimetal, one has

$$\gamma = 0, \quad S_{ex} = 2\pi \frac{[\zeta - \varepsilon_d(p_3^{ex})]^2}{\alpha|\cos[\theta(p_3^{ex})]|}, \quad m_* = \frac{2[\zeta - \varepsilon_d(p_3^{ex})]}{\alpha|\cos[\theta(p_3^{ex})]|}, \quad \frac{\partial^2 S}{\partial p_z^2} = \frac{1}{(\cos[\theta(p_3^{ex})])^2} \frac{\partial^2 S}{\partial p_3^2}. \qquad (44)$$

Inserting these expressions into Eq. (41), we arrive at formula (40).

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