De Haas-van Alphen effect in two- and quasi two-dimensional metals and superconductors

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Abstract

An analytical form of the quantum magnetization oscillations (de Haas-van Alphen effect) is derived for two- and quasi two-dimensional metals in normal and superconducting mixed states. The theory is developed under condition $\mu/\omega_c \gg 1$ (μ is the chemical potential and ω_c the cyclotron frequency), which is proved to be valid for using grand canonical ensemble in the systems of low dimensionality. Effects of impurity, temperature, spin-splitting and vortex lattice - in the case of superconductors of type II -, are taken into account. Contrary to the three dimensional case, the oscillations in sufficiently pure systems of low dimensionality and at sufficiently low temperatures are characterized by a saw-tooth wave form, which smoothened with temperature and concentration of impurities growth. In the normal quasi two-dimensional systems, the expression for the magnetization oscillations includes an extra factor expressed through the transfer integral between the layers. The additional damping effect due to the vortex lattice is found. The criterion of proximity to the upper critical field for the observation of de Haas-van Alphen effect in the superconducting mixed state is established.

1 Introduction

De Haas-van Alphen (dHvA) effect is well known to be a powerful tool to get information on the shape of the Fermi surface of normal metals. In contrast to three-dimensional (3D) metals where the experimental observations have well established base given by the Lifshitz-Kosevich (1956) theory, there is no unanimously acknowledged and used theory applicable to 2D or quasi 2D layered materials. Schoenberg (1984) introduced an expression for magnetic oscillations in 2D metals where he put phenomenologically the effect of temperature. Effect of impurities is not considered, although it can be important. There are two essential features of dHvA effect in 2D case commonly believed differing it from its 3D counterpart :

(i) The sharp saw-tooth like shape of dHvA signal at sufficiently low temperatures.

(ii) Strong dependence of the chemical potential on the magnetic field, that is why the proper derivation has to be done in the canonical ensemble with fixed number of particles.

To make clear this subject we note that the property (i) takes place in 2D case both at constant number of particles or at constant chemical potential so long we are in the low temperature $T \ll \omega_c$ and high purity region $\Gamma < \omega_c$. Here, ω_c is the distance between Landau levels, Γ is the width of level. As for property (ii) its validity is directly related to the concentration of the charge carriers we deal with. For low enough concentrations when $\omega_c \sim \varepsilon_F = \frac{\pi n}{m^*}$ (*n* is the electron density and m^* is the effective mass), the oscillations of the chemical potential μ with magnetic field are important and one has to proceed with the calculations in canonical ensemble (see the papers (Jauregui *et al.* 1990, Harrison*et al.* 1996, Grigoriev and Vagner 1999, Nakano 1998)). On the contrary under the condition $\mu \approx \varepsilon_F = \frac{\pi n}{m^*} \gg \omega_c$ the oscillations of the chemical potential are small and one may work making use the grand canonical ensemble as in 3D case. The analytical theory of dHvA effect in 2D and layered quasi 2D metals taking into account the effects of temperature, impurities and spin-splitting is developed in the first part of this paper. It is proved that the grand canonical ensemble is well accurate for systems of low dimensionality in the limit $\mu/\omega_c \gg 1$. In pure case and at zero temperature the oscillations have the saw-tooth shape. The finite temperature as well as the finite amount of impurities (even at zero temperature) lead to the natural smoothening of the oscillations. The results of calculations (but not the calculations themselves) of magnetization oscillations in frame of grand canonical ensemble for quasi 2D spinless and perfect crystal model can be found in the paper (Nakano 1998). If do not take in mind the opposite sign of magnetization (it is probably due to a misprint) they coincide with ours taken in the absence of impurities and spin paramagnetism. The recent experimental studies (Wosnitsa *et al.* 2000) in several organic compounds demonstrate magnetization oscillations behavior similar to that should be in the systems with fixed chemical potential.

In a parallel direction to the study of dHvA effect in the normal low dimensional systems, the possibility of doing quantum oscillations measurements in the superconducting mixed state has been recognized after its first manifestation by Graebner and Robbins (Graebner and Robbins 1976). During the last ten years, dHvA effect has already been observed both in mixed state and normal state of many types of superconductors like $NbSe_2$ (Haworth *et al.* 1999), Nb_3Sn (Harrison *et al.* 1994), V_3Si (Corcoran *et al.* 1994), YNi_2B_2C (Goll *et al.* 1996, Terashima *et al.* 1997), $CeRu_2$ (Hedo *et al.* 1998), UPd_2Al_3 (Haga *et al.* 1999), URu_2Si_2 (Ohkuni *et al.* 1999), $\kappa - (BEDT - TTF)_2Cu(NCS)_2$ (Sasaki *et al.* 1998). Apart the low temperature

$$T < \omega_c \sim \frac{eH_{c2}}{mc} \sim \frac{T_c^2}{\varepsilon_F}$$

the condition of observation of dHvA effect in the superconducting mixed state consists of ultra purity of the samples

$$l > \frac{v_F}{\omega_c} \sim \frac{\varepsilon_F}{T_c} \xi_0.$$

Here l is the mean free path of quasiparticles, ξ_0 is the coherence length. Both of these demands mean that all enumerated above samples of materials are ultra clean and at the same time very strong type-II superconductors with high upper critical field value. The latter is provided by the higher critical temperature and the lower Fermi energy than in ordinary type-II superconductors.

The main observation consists of that the frequency of oscillations in the mixed state remains the same but the amplitude decreases with decreasing field more rapidly than in the normal state. The effect becomes unobservable at fields several times smaller than H_{c2} but still much larger than the thermodynamic critical field $H_c = H_{c2}/\kappa$. Here κ is the Ginzburg-Landau parameter, which is of the order of 20-30 typically for observations of dHvA in mixed state materials. That means the distance between the vortices is of the order of its core diameter in the whole region of the observation. Hence the latter can be considered as vicinity of the upper critical field where the Abrikosov solution for the vortex lattice serves as a good approximation.

Another important observation (Goll *al.* 1996; T.Terashima *et al.* 1997) is that dHvA effect in the superconducting mixed state persists below the upper critical field not for all but for the electron orbits with relatively smaller radius (or cross section area).

Numerous theoretical studies were done to understand the effect of vortex lattice. The essential point here is a nondiagonality of the order parameter matrix in the Landau representation preventing a simple derivation of the quasiparticle energy spectrum in the mixed state. The intention to avoid of this problem leads to the idea to work with oversimplifyed BCS type spectrum (Miller and Gyorffy 1995; Dukan and Tesanovich 1995); Gvozdikov and Gvozdikova 1998), which is valid either in the quasiclassical region far below of H_{c2} where the dHvA effect does not take place or in ultra quantum limit with only few filled Landau levels. In the latter case there are however doubts as in the applicability of the BCS theory as in the existance of the superconductivity.

It should be mentioned also an attempt to develope a theory for anisotropic superconductors with nodes in the gap on the Fermi surface far below H_{c2} where a vortex core radius is much smaller than the distance between vortices, and one can assume the space constancy of the order parameter modulus (Gorkov and Schrieffer 1998). As we pointed above it does not corresponds to the observations region.

The proper derivation has been proposed by K.Maki (1991) and M.Stephen (1992). There were established an additional attenuation of the dHvA amplitude in the superconducting mixed state. The order parameter has been determined self-consistently by M.Stephen that has allowed to point out the field interval near H_{c2} where the effect is accessible for observation. The mentioned results were obtained in neglect by the nondiagonal elements of the self-energy matrix , or sort of random vortex lattice potential approximation has been used.

Somethat later the numerical calculations for two-dimensional electron system has been performed (Norman and MacDonald 1996; Bruun, Nicos Nicopoulos and Johnson 1997).

Another type of analitical results (with less rapid attenuation of dHvA signal with decreasing of magnetic field in the superconducting region) were represented in the paper (Zhuravlev et al, 1997), where so called strict phase coherence approach has been applied. Although the latter has definitive theoretical interest it seems to be less realistic than the random vortex lattice potential approximation has been used in the Stephen's paper.

The treatments (Stephen 1992, Norman and McDonald 1996, Bruun, Nicos Nicopoulos and Johnson 1997, Zhuravlev et al, 1997) were limited by the condition $T > \omega_c/2\pi^2$ which is necessary for the convergency at low temperatures. The spreading of the theory on the low temperature region $\omega_c > \Gamma > T$ by an introduction of the width of the Landau levels Γ originating of impurity scattering has been done in the papers (Vavilov and Mineev 1997; 1998; Mineev 1999). It was shown that a superconducting state is gapless in the mixed state region below the upper critical field if

$$\frac{H_{c2} - H}{H_{c2}} < \sqrt{\frac{\omega_c}{\varepsilon_F}} \ln \frac{\varepsilon_F}{\omega_c},\tag{1}$$

where ε_F/ω_c is the number of Landau levels below the Fermi surface at $H = H_{c2}$. This field interval is negligible for any typical type-II superconductor. However for those particular ultraclean materials with very high H_{c2} and very small ε_F , where dHvA effect in the superconducting mixed state have been observed, the value of $\sqrt{\varepsilon_F/\omega_{c2}}$ is of the order of or even smaller than ten and the presented theory has sizable region of applicability below the upper critical field. In this region, the oscillatory contribution to the density of states and the damping of the amplitude of the magnetization oscillation in the superconducting state were found.

It also important to note that amount of Landau levels below the Fermi energy is different for the different bands (ε_F in (1) should be diminished on the value of energy at the center of the band under consideration). That is why the condition (1) is less restrictive for the electron orbits with smaller radius or cross section area. This fact is in correspondence with the observations mentioned above.

In the unconventional superconducting states where the lines of extremal cross-section of Fermi-surface by the plane perpendicular to magnetic field coincide with lines of zeros of the order parameter the amplitude of the magnetization oscillations is practically the same as in a normal state. In the superconducting state with an other distribution of zeros the damping of dHvA oscillations corresponds qualitatively to the ordinary superconductivity.

The further development of the theory of the dHvA effect in the superconducting mixed state, has been done in the paper (Mineev 2000). In three-dimensional isotropic model there was analitically derived the Landau expansion for the free energy of the superconducting mixed state near the upper critical field in powers of the square modulus of the order parameter averaged over Abrikosov lattice with Landau quantization of the quasiparticle energy taken into consideration.

The condition of the valitity of such the expansion were established and it is given by the formula (1).

As in the normal metal the oscillating with magnetic field terms represent the tiny corrections to the nonoscillating free energy of the superconducting state. However they are fast oscillating functions of the ratio $2\pi\varepsilon_F/\omega_c$. Becouse of that after the differentiation over the magnetic field $M = -\left(\frac{\partial F}{\partial H}\right)_{\mu,T}$ the oscillating part of the magnetization in the superconducting mixed state proves to be even larger than corresponding nonoscillating part of magnetization.

The analytical theory of the dHvA effect in the superconducting mixed state in the vicinity of the upper critical field for 2D and quasi 2D layered superconductors is developed in the second part of the present article. Our treatment follows the paper (Mineev 2000) where the corresponding calculations have been performed for 3D superconductors.

2 De Haas-van Alphen effect in two-dimensional normal metals

In order to derive the magnetization M, it is necessary to calculate first the free energy F which is related to the thermodynamic potential Ω in grand canonical ensemble by¹

$$F = \Omega + \mu N \tag{2}$$

with

$$\Omega = -T \int_0^\infty g(\varepsilon) \ln(1 + e^{\frac{\mu - \varepsilon}{T}}) \, d\varepsilon \tag{3}$$

where μ is the chemical potential of the system, N is the number of electrons per unit volume and $q(\varepsilon)$ is the density of states in presence of the magnetic field H and the impurities.

2.1 Density of States

The latter can be achieved from the imaginary part of the space averaged single-electron Green's function $\bar{G}(\varepsilon)$ using the relation

$$g(\varepsilon) = -\frac{1}{\pi} sign(\varepsilon - \mu) \Im \bar{G}(\varepsilon).$$
(4)

We then follow the proceeding of Bychkov (1961), who has dealt with the effect of impurities in 3D metals under magnetic field using a perturbation method. The broadening of each Landau level into the energy distribution with Lorenz density of states has been found in this paper supposed to be not so bad approximation in 2D and quasi 2D cases apparently valid in not very strong magnetic fields (see Prange 1987). So, we shall use the Green's function in the following form

$$\bar{G}(\varepsilon) = \sum_{m} \frac{1}{\varepsilon - E_m + i\Gamma sign(\varepsilon - \mu)}$$
(5)

where m specifies the quantum numbers, Γ the width of Landau's levels due to impurity scattering ($\Gamma = 1/2\tau$ with τ a mean free time of quasiparticles) and E_m the energy spectrum of the stationary states in absence of impurities. The quantum numbers depend on the dimensionality of the considered system : for the 2D case, the set of quantum numbers m includes the magnetic quantum number n of the Landau's levels, a wave number k_y which is connected with the center of the orbit of the electrons, and the spin $\sigma = \pm 1$; for the 3D

¹Planck's constant \hbar , the Boltzmann's constant k_B and the ratio of electron charge |e| to the velocity of light c are chosen to be unity throughout the paper

case, we have in addition the momentum k_z . The field **H** is directed along the z axis, that is in 2D case perpendicular to the conducting plane. The energies are :

$$E_{n,k_z,\sigma}^{3d} = \omega_c (n + \frac{1}{2}) + \frac{k_z^2}{2m} + \sigma \mu_e H,$$
(6)

$$E_{n,\sigma}^{2d} = \omega_c (n + \frac{1}{2}) + \sigma \mu_e H \tag{7}$$

One needs to remember that all the energies should be counted from the energy ε_b at the center of the considered band. Keeping in mind this circumstance we shall shift the chemical potential in final formulas on this value. The expression for the single Green's function for a given spin σ becomes in the 2D case

$$\bar{G}^{\sigma}(\varepsilon) = N_0 \omega_c \sum_{n=0}^{\infty} \frac{1}{\varepsilon - \omega_c (n + \frac{1}{2}) - \sigma \mu_e H + i \Gamma sign(\varepsilon - \mu)}.$$
(8)

Here $N_0 = \frac{m}{2\pi}$ is the normal metal electron density of states per one spin projection and μ_e is the electron's magnetic moment. The expression (8) is divergent. In fact, it is the case only for the real part of $\bar{G}^{\sigma}(\varepsilon)$; the imaginary part, which we have to calculate next, is convergent

$$\Im \bar{G}^{\sigma}(\varepsilon) = N_0 \omega_c \sum_{n=0}^{+\infty} \frac{-\Gamma sign(\varepsilon - \mu)}{(\varepsilon - \omega_c (n + \frac{1}{2}) - \sigma \mu_e H)^2 + \Gamma^2}.$$
(9)

The Poisson's summation formula

$$\sum_{n=0}^{\infty} f(n) = \sum_{l=-\infty}^{+\infty} \int_{a}^{+\infty} f(t) e^{-2\pi i lt} dt$$

where a is a number between -1 and 0, can now be used properly. Writing $\varepsilon = \xi + \mu$, changing variable t to $x = t - \frac{\mu}{\omega_c \mu}$, and then setting the lower limit of the integral equal to $-\infty$ since we consider the limit $\frac{\omega_c}{\omega_c} \gg 1$, we get

$$\Im \,\bar{G}^{\sigma}(\varepsilon) = -\pi N_0 sign\xi + \Im \,\bar{G}^{\sigma}_{osc}(\varepsilon) \tag{10}$$

with

$$\Im \,\bar{G}^{\sigma}_{osc}(\varepsilon) = -N_0 \omega_c \Gamma sign\xi \sum_{l=-\infty,\neq 0}^{+\infty} e^{-2\pi i l \frac{\mu}{\omega_c}} \int_{-\infty}^{+\infty} \frac{e^{-2\pi i l x} \, dx}{(\xi - \omega_c (x + \frac{1}{2}) - \sigma \mu_e H)^2 + \Gamma^2}.$$
 (11)

The first term in the right hand side of equation (10) comes from the contribution of l = 0 in the sum and corresponds to the result in absence of field. The other contributions $l \neq 0$ give an oscillatory part depending on the field. The remaining integration is quite straightforward by a residue calculation and yields

$$\Im \,\bar{G}_{osc}^{\sigma}(\varepsilon) = 2\pi sign(\varepsilon - \mu) N_0 \sum_{l=1}^{+\infty} (-1)^{l+1} \cos\left(2\pi l \frac{(\varepsilon - \sigma \mu_e H)}{\omega_c}\right) \, e^{-2\pi l \frac{\Gamma}{\omega_c}}.$$
 (12)

From relation (4), we get directly the searched density of states, after summing up the two spin states

$$g^{2d}(\varepsilon) = 2N_0 \left[1 + 2\sum_{l=1}^{+\infty} (-1)^l \cos(2\pi l \frac{\varepsilon}{\omega_c}) \cos(2\pi l \frac{\mu_e H}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}} \right].$$
(13)

2.2 Chemical potential

Making use of equation (3), the oscillatory part of the thermodynamic potential Ω is performed by an integration by parts and by the change of variable $x = \frac{(\varepsilon - \mu)}{T}$

$$\Omega_{osc}^{2d} = 2N_0 T\omega_c \sum_{l=1}^{+\infty} \frac{(-1)^{l+1}}{l} e^{-2\pi l \frac{\Gamma}{\omega_c}} \cos(2\pi l \frac{\mu_e H}{\omega_c}) \frac{1}{\pi} \int_{-\frac{\mu}{T}}^{+\infty} \frac{\sin(2\pi l \frac{(\mu+Tx)}{\omega_c})}{1+e^x} dx.$$
(14)

The lower limit of the integral may be set equal to $-\infty$ since in our investigation we have the condition $\mu \gg T$. Using the value of the integral

$$\int_{-\infty}^{+\infty} \frac{e^{i\alpha y}}{1+e^y} \, dy = -\frac{i\pi}{\sinh(\alpha \pi)}$$

we find at last

$$\Omega_{osc}^{2d} = 2N_0 T \omega_c \sum_{l=1}^{+\infty} \frac{(-1)^l}{l} e^{-2\pi l \frac{\Gamma}{\omega_c}} \cos(2\pi l \frac{\mu}{\omega_c}) \frac{\cos(2\pi l \frac{\mu_e H}{\omega_c})}{\sinh(\frac{2\pi^2 l T}{\omega_c})}.$$
(15)

The nonoscillatory part of the thermodynamic potential gives on its side

$$\Omega_0^{2d} = -N_0 \mu^2. (16)$$

The number of electrons is defined by $N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,H}$ and thus

$$N = 2N_0\mu + 4\pi N_0 T \sum_{l=1}^{+\infty} (-1)^l \frac{\cos(2\pi l \frac{\mu_e H}{\omega_c})}{\sinh(\frac{2\pi^2 l T}{\omega_c})} \sin(2\pi l \frac{\mu}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}}.$$
 (17)

This formula determines of the number of particles as the function of (H, T) at fixed μ . On the other hand one can consider it as the equation for the chemical potential as the function of (H, T) at fixed number of particles. Recognizing the Fermi energy

$$\varepsilon_F = \frac{N}{2N_0} \tag{18}$$

one can rewright this equation as

$$\mu = \varepsilon_F + \frac{\omega_c}{\pi} \sum_{l=1}^{+\infty} \frac{(-1)^{l+1}}{l} \frac{\lambda_l}{\sinh \lambda_l} \sin(2\pi l \frac{\mu}{\omega_c}) \cos(2\pi l \frac{\mu_e H}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}}$$
(19)

with

$$\lambda_l = \frac{2\pi^2 lT}{\omega_c}.$$

We see that at $\varepsilon_F \gg \omega_c$ the second oscillating term represent the small correction to the const value of chemical potential. On the other hand the expression (11) has been obtained in neglect of terms of the order of ω_c/μ . That is why it would be out of limits our accuracy to keep the difference between the chemical potential and Fermi energy in the right hand side of (19). So, finally we get

$$\mu = \varepsilon_F + \frac{\omega_c}{\pi} \sum_{l=1}^{+\infty} \frac{(-1)^{l+1}}{l} \frac{\lambda_l}{\sinh \lambda_l} \sin(2\pi l \frac{\varepsilon_F}{\omega_c}) \cos(2\pi l \frac{\mu_e H}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}}.$$
 (20)

It is worth to remind here that in real crystal one should to shift all the energies on the energy in center of band: $\mu \to \mu - \varepsilon_b$, $\varepsilon_F \to \varepsilon_F - \varepsilon_b$.

At zero temperature, ignoring for brevity the spin splitting and summing up over l, we find a simple expression

$$\mu = \varepsilon_F + \frac{\omega_c}{\pi} \arctan\left(\frac{\sin(2\pi\frac{\varepsilon_F}{\omega_c})}{\cos(2\pi\frac{\varepsilon_F}{\omega_c}) + e^{2\pi\frac{\Gamma}{\omega_c}}}\right)$$
(21)

which is obviously has at $\Gamma = 0$ saw-tooth shape. At any finite Γ , the oscillations of the chemical potential are smooth. For instance for $2\pi\Gamma/\omega_c \ge 1$

$$\mu = \varepsilon_F + \frac{\omega_c}{\pi} \sin(2\pi \frac{\varepsilon_F}{\omega_c}) e^{-2\pi \frac{\Gamma}{\omega_c}}.$$
(22)

On this stage one should stress ones more that all the results has been obtained here at the condition $\mu/\omega_c \gg 1$.

2.3 Magnetization

The magnetization $M = -\left(\frac{\partial\Omega}{\partial H}\right)_{\mu,T}$ can be found from the relation (14). Keeping only the preponderant terms and ignoring as before the small difference between μ and ε_F in the arguments of oscillating harmonics², we obtain

$$M_{n,osc}^{2d} = \sum_{l=1}^{+\infty} M_l^{2d} = N_0 \frac{2}{\pi} \frac{\omega_c}{H} \varepsilon_F \sum_{l=1}^{+\infty} \frac{(-1)^{l+1}}{l} \frac{\lambda_l}{\sinh \lambda_l} \sin(2\pi l \frac{\varepsilon_F}{\omega_c}) \cos(2\pi l \frac{\mu_e H}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}}.$$
 (23)

This formula without impurities factor corresponds to the intuitive formula given by Schoenberg (1984). After (20) and (23) we notice that at $\varepsilon_F \gg \omega_c$ the magnetization is directly related to the oscillating part of μ by

$$M_{n,osc}^{2d} = \frac{N}{H}\mu_{osc} = M_0 \frac{\mu_{osc}}{\omega_c}.$$
(24)

This result, which is valid at any temperature smaller than the ε_F , generalizes that was given in the recent paper (Itskovsky, Maniv and Vagner 2000) for the range of temperature $T \leq \omega_c$.

For T=0, this expression is simplified since a summation over the integers l is possible. Without spin-splitting, we have

$$M_{n,osc}^{2d} = \frac{2N_0}{\pi} \frac{\omega_c}{H} \varepsilon_F \arctan\left(\frac{\sin(2\pi \frac{\varepsilon_F}{\omega_c})}{\cos(2\pi \frac{\varepsilon_F}{\omega_c}) + e^{2\pi \frac{\Gamma}{\omega_c}}}\right)$$
(25)

and with spin-splitting

$$M_{n,osc}^{2d} = \frac{N_0}{\pi} \frac{\omega_c}{H} \varepsilon_F \arctan\left(\frac{\sin(4\pi\frac{\varepsilon_F}{\omega_c}) + 2\sin(2\pi\frac{\varepsilon_F}{\omega_c})\cos(2\pi\frac{\mu_e H}{\omega_c})e^{2\pi\frac{\Gamma}{\omega_c}}}{\cos(4\pi\frac{\varepsilon_F}{\omega_c}) + 2\cos(2\pi\frac{\varepsilon_F}{\omega_c})\cos(2\pi\frac{\mu_e H}{\omega_c})e^{2\pi\frac{\Gamma}{\omega_c}} + e^{4\pi\frac{\Gamma}{\omega_c}}}\right).$$
 (26)

For $2\pi\Gamma/\omega_c \geq 1$, this yields

$$M_{n,osc}^{2d} = \frac{2N_0}{\pi} \frac{\omega_c}{H} \varepsilon_F \sin(2\pi \frac{\varepsilon_F}{\omega_c}) \cos(2\pi \frac{\mu_e H}{\omega_c}) e^{-2\pi \frac{\Gamma}{\omega_c}}.$$
 (27)

²The restoration of the oscillating difference $\mu - \varepsilon_F$ would be resulted in the additional frequences in Fourier spectrum of the magnetization which certainly present when the ratio ω/ε_F is not small. One should stress however that both formulas for the chemical potential and for the magnetization are derived here by making use the expression for the density of states have been found in the neglect of terms of the order of ω_c/ε_F and keeping of such the terms in the oscillating arguments would be out the limits of accuracy we used.

3 De Haas-van Alphen effect in quasi two-dimensional normal metals

In layered metals, the simplest spectrum for electrons is

$$E_{n,k_z,\sigma} = \omega_c (n + \frac{1}{2}) - 2t \cos(k_z d) + \sigma \mu_e H.$$
 (28)

The parameter t is the transfer integral along the z axis, d is the distance between the layers. Here the field \mathbf{H} is perpendicular to the layers. More generally, in a tilted magnetic field, the spectrum energy is quantized as (Yamaji 1989)

$$E_{n,k_z,\sigma} = \omega_c \cos\theta \left(n + \frac{1}{2}\right) - 2t J_0(k_F d \tan\theta) \cos(k_z d) + \sigma \mu_e H$$
⁽²⁹⁾

where J_0 is the Bessel's function of zero order and k_F is the momentum at the Fermi's surface. For convenience, we will work with spectrum (28). The corresponding generalization for the case of finite tilting is easy with simple substitution of the angle dependent parameters. According to (5), the space averaged Green's function becomes henceforth

$$\bar{G}^{\sigma}(\varepsilon) = \frac{N_0 \omega_c}{2\pi d} \sum_{n=0}^{\infty} \int_{-\pi}^{\pi} \frac{d\psi}{\varepsilon - \omega_c (n + \frac{1}{2}) - \sigma \mu_e H + 2t \cos \psi + i\Gamma sign(\varepsilon - \mu)}.$$
 (30)

Here we consider that $t \leq \text{or} \sim \omega_c$ so that roughly speaking only the modulation of one Landau level is taken into account. For $t \gg \omega_c$, many Landau levels play a role and we can do the following approximation

$$-(n+\frac{1}{2}) + \frac{2t}{\omega_c}\cos\psi \approx -(n+\frac{1}{2}) + \frac{2t}{\omega_c}(1-\frac{(k_zd)^2}{2}).$$

In this limit, we are again in the 3D case. Next, we proceed exactly like previously using the Poisson's summation formula. The density of states includes then an additional Bessel function factor

$$g^{q2d}(\varepsilon) = \frac{2N_0}{d} \left[1 + 2\sum_{l=1}^{+\infty} (-1)^l \cos(2\pi l \frac{\varepsilon}{\omega_c}) J_0(2\pi l \frac{2t}{\omega_c}) \cos(2\pi l \frac{\mu_e H}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}} \right]$$
(31)

with

$$J_0(z) = \frac{1}{2\pi} \int_{-\pi}^{+\pi} e^{2\pi i z \cos \psi} \, d\psi$$

and the oscillatory part of the thermodynamic potential becomes

$$\Omega_{osc}^{q2d} = 2\frac{N_0}{d}T\omega_c \sum_{l=1}^{+\infty} \frac{(-1)^l}{l} \frac{\cos(2\pi l\frac{\mu}{\omega_c})}{\sinh(\lambda_l)} J_0(2\pi l\frac{2t}{\omega_c}) \cos(2\pi l\frac{\mu_e H}{\omega_c}) e^{-2\pi l\frac{\Gamma}{\omega_c}}.$$
 (32)

Thus

$$M_{n,osc}^{q2d} = \frac{N_0}{d} \frac{2}{\pi} \frac{\omega_c}{H} \mu \sum_{l=1}^{+\infty} \frac{(-1)^{l+1}}{l} \frac{\lambda_l}{\sinh \lambda_l} \cos(2\pi l \frac{\mu_e H}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}} \\ \times \left\{ \sin(2\pi l \frac{\mu}{\omega_c}) J_0(2\pi l \frac{2t}{\omega_c}) + \frac{2t}{\mu} \cos(2\pi l \frac{\mu}{\omega_c}) J_1(2\pi l \frac{2t}{\omega_c}) \right\}$$
(33)

where $J_1(z) = -J'_0(z)$ is the Bessel's function of first order.

Assuming that the transfer energy t is much smaller than the Fermi energy ε_F , we obtain

$$M_{n,osc}^{q2d} = \frac{N_0}{d} \frac{2}{\pi} \frac{\omega_c}{H} \mu \sum_{l=1}^{+\infty} \frac{(-1)^{l+1}}{l} \frac{\lambda_l}{\sinh \lambda_l} \sin(2\pi l \frac{\mu}{\omega_c}) J_0(2\pi l \frac{2t}{\omega_c}) \cos(2\pi l \frac{\mu_e H}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}}.$$
 (34)

Here we remind that in reality the chemical potential μ has to be reduced on the energy of the band center $\mu \to \mu - \varepsilon_b \approx \varepsilon_F - \varepsilon_b$. Without spin-splitting and impurities factor, this result is the same as given in (Nakano 1998) except the opposite sign probably due to a misprint. The extra factor $J_0(2\pi l \frac{2t}{\omega_c})$ in this expression induces a rich behavior for the manifestly field dependent amplitude of the harmonics. In formal limit $2t \gg \omega_c$,

$$J_0(z) \sim \sqrt{\frac{2}{\pi z}} \cos(z - \frac{\pi}{4})$$

and thus we return back to expression closed to Lifshitz-Kosevich result (Lifshits and Kosevich 1956) for the amplitude of the harmonics. For $2t \ll \omega_c$, $J_0(z) \sim 1$ and we find again the 2D expression (23).

4 De Haas-van Alphen effect in mixed state of two- and quasi two-dimensional superconductors

In this section, we want to determine the effect of the low-dimensionality on the additional damping factor due to the vortex lattice. In this purpose, we follow the work (Mineev 2000) (and also take the same notations) where the theory of dHvA effect for 3D metals in the superconducting mixed state has been developed, and adapt it to 2D and quasi 2D systems. It should be mentioned that under 2D systems we shall imply 3D layered crystals with negligibly small interaction between layers, such that the mixed state in the magnetic field perpendicular to the layers represents Abrikosov but not Pearl vortex lattice. The treatment of the problem is carried out in the framework of the Gorkov's formalism for a conventional superconductor.

4.1 Free energy

The free energy density in mixed state near the upper critical field H_{c2} is developed in powers of the square modulus of the order parameter averaged over the Abrikosov's lattice (Mineev 2000)

$$F_s - F_n = \alpha \Delta^2 + \frac{\beta}{2} \Delta^4 \tag{35}$$

where

$$\alpha = \frac{1}{g} - \int e^{-\frac{H\rho^2}{2}} K_2(\mathbf{R}) \, d\mathbf{R} \tag{36}$$

and

$$\beta = \frac{1}{V} \int f^*(\mathbf{r_1}) f(\mathbf{r_2}) f^*(\mathbf{r_3}) f(\mathbf{r_4}) K_4(\mathbf{r_1}, \mathbf{r_2}, \mathbf{r_3}, \mathbf{r_4}) \, d\mathbf{r_1} \, d\mathbf{r_2} \, d\mathbf{r_3} \, d\mathbf{r_4}.$$
(37)

Here g is the constant of the pairing interaction, $\rho^2 = R^2 - Z^2$,

$$f(\mathbf{r}) = 2^{1/4} \sum_{\nu = integer} \exp\left(i\frac{2\pi\nu}{a}y - \left(\frac{x}{\lambda} + \frac{\pi\nu}{a}\lambda\right)^2\right)$$

is the Abrikosov square lattice solution for the order parameter where the elementary cell edge a is such that $a^2 = \pi \lambda^2$ and $\lambda = H^{-1/2}$ is the magnetic length and Δ is the order parameter amplitude.

The functions K_2 and K_4 have the following expressions :

$$K_2(\mathbf{R}) = \frac{1}{2} \sum_{\sigma=\pm 1} T \sum_{\nu} \tilde{G}^{\sigma}(\mathbf{R}, \tilde{\omega}_{\nu}) \tilde{G}^{-\sigma}(\mathbf{R}, -\tilde{\omega}_{\nu}), \qquad (38)$$

$$G^{\sigma}(\mathbf{r}_1, \mathbf{r}_2, \tilde{\omega}_{\nu}) = \exp\left(i \int_{\mathbf{r}_1}^{\mathbf{r}_2} \mathbf{A}(\mathbf{s}) \, d\mathbf{s}\right) \tilde{G}^{\sigma}(\mathbf{r}_1 - \mathbf{r}_2, \tilde{\omega}_{\nu}),\tag{39}$$

$$K_4(\mathbf{r_1}, \mathbf{r_2}, \mathbf{r_3}, \mathbf{r_4}) = \frac{1}{2} \sum_{\sigma=\pm 1} T \sum_{\nu} G^{\sigma}(\mathbf{r_1}, \mathbf{r_2}, \tilde{\omega_{\nu}}) G^{-\sigma}(\mathbf{r_2}, \mathbf{r_3}, -\tilde{\omega_{\nu}}) G^{\sigma}(\mathbf{r_3}, \mathbf{r_4}, \tilde{\omega_{\nu}}) \times G^{-\sigma}(\mathbf{r_1}, \mathbf{r_4}, -\tilde{\omega_{\nu}}), \qquad (40)$$

$$\widetilde{\omega}_{\nu} = \omega_{\nu} + \Gamma sign\omega_{\nu}, \qquad \omega_{\nu} = \pi T(2\nu + 1).$$
(41)

To obtain this formula, it is assumed that the magnetic field is uniform and coincides with external field, which is a good approximation in the vicinity of H_{c2} for superconductors with large Ginzburg-Landau parameter.

The coefficients α and β , which depend on the dimensionality of the system by way of the Green's functions, are calculated respectively in appendix A and in appendix B in the semi-classical approximation $\frac{\mu}{\omega_c} \gg 1$. They consist of a smooth function and a fast oscillating function of the magnetic field :

$$\alpha(H,T) = \bar{\alpha}(H,T) + \alpha_{osc}(H,T), \qquad (42)$$

$$\beta(H,T) = \bar{\beta}(H,T) + \beta_{osc}(H,T).$$
(43)

For a two-dimensional system, we find

$$\bar{\alpha}^{2d}(H,T) = \frac{N_0}{2} \frac{H - \bar{H}_{c2}^{2d}(T)}{H_{c2g}^{2d}}$$
(44)

where $\bar{H}_{c2}(T)$ is the upper critical field at low temperatures averaged over the oscillations,

$$\alpha_{osc}^{2d}(H,T) = -4\pi^{3/2} N_0 \frac{T}{\sqrt{\mu\omega_c}} \sum_{l=1}^{+\infty} (-1)^l \cos(2\pi l \frac{\mu}{\omega_c}) \cos(2\pi (l+2) \frac{\mu_e H}{\omega_c}) \times \frac{e^{-2\pi (l+2) \frac{\Gamma}{\omega_c}}}{\sinh \lambda_{l+2}}$$
(45)

and

$$\bar{\beta}^{2d}(H,T=0) = N_0 \frac{\omega_c}{16\pi\mu} \frac{\Gamma^2 - (\mu_e H)^2}{(\Gamma^2 + (\mu_e H)^2)^2} \approx N_0 \frac{\omega_c}{16\pi\mu\Gamma^2}$$
(46)

which is valid for $\mu_e H < \Gamma < \omega_c$,

$$\beta_{osc}^{2d}(H,T=0) = N_0 \frac{\omega_c}{2\pi\mu\Gamma^2} \sum_{l=1}^{+\infty} (-1)^l \cos(2\pi l \frac{\mu}{\omega_c}) I(2\pi l \frac{\Gamma}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}}$$
(47)

where $I(x) = \int_0^\infty \left[\frac{1}{(y+1)^3} + \frac{x}{(1+y)^2}\right] e^{-xy} dy$ is a bounded function. Minimization of the free energy over Δ yields

$$F_s = F_n - \frac{\alpha^2}{2\beta}.\tag{48}$$

4.2 Magnetization

Magnetization is given by $M_s = -\frac{\partial F_s}{\partial H}$. In the differentiation we keep only the fast oscillating terms

$$M_{s,osc} \simeq M_{n,osc} + \frac{\bar{\alpha}}{\bar{\beta}} \frac{\partial \alpha_{osc}}{\partial H} - \frac{\bar{\alpha}^2}{2\bar{\beta}^2} \frac{\partial \beta_{osc}}{\partial H}.$$
(49)

Here $M_{n,osc}$ is the oscillating part of the normal metal magnetization calculated previously (see equation (23)). Like in the 3D case (Mineev 2000), at $4\pi\Gamma \sim \omega_c$ the following inequality takes place

$$|M_{n,osc}| > |\frac{\bar{\alpha}}{\bar{\beta}} \frac{\partial \alpha_{osc}}{\partial H}| > |-\frac{\bar{\alpha}^2}{2\bar{\beta}^2} \frac{\partial \beta_{osc}}{\partial H}|$$
(50)

until the new more restrictive than in the 3D case (see (1)) condition :

$$\frac{\bar{H}_{c2}(T) - H}{H_{c2o}} < \left(\frac{\omega_c}{\mu}\right)^{1/2}.$$
(51)

With the previous condition we keep also only the first two terms and obtain for the oscillating part of the magnetization

$$M_{s,osc}^{2d} = M_{n,osc}^{2d} + \frac{\bar{\alpha}}{\bar{\beta}} \frac{\partial \alpha_{osc}}{\partial H} = \sum_{l=1}^{+\infty} M_{nl}^{2d} M_{sl}^{2d},$$
(52)

where

$$M_{nl}^{2d} = N_0 \frac{2}{\pi} \frac{\omega_c}{H} \mu \frac{(-1)^{l+1}}{l} \frac{\lambda_l}{\sinh \lambda_l} \sin(2\pi l \frac{\mu}{\omega_c}) \cos(2\pi l \frac{\mu_e H}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}}$$
(53)

and

$$M_{sl}^{2d} = 1 - \sqrt{\pi} \left(\frac{4\pi\Gamma}{\omega_c}\right)^2 \sqrt{\frac{\mu}{\omega_c}} \frac{\bar{H}_{c2-} - H}{H_{c2o}} \frac{l^2 \lambda_{l+2} \sinh \lambda_l}{(l+2)\lambda_l \sinh \lambda_{l+2}} \\ \times \frac{\cos(2\pi(l+2)\frac{\mu_e H}{\omega_c})}{\cos(2\pi l \frac{\mu_e H}{\omega_c})} e^{-\frac{4\pi\Gamma}{\omega_c}}$$
(54)

with

$$\lambda_l = \frac{2\pi^2 lT}{\omega_c}.$$

All the previous calculations can be done in the same way for a quasi-two dimensional system. We give only the final result

$$M_{sl}^{q2d} = M_{sl}^{2d}.$$
 (55)

The field interval (51) in which the results (52), (53), (54) are valid is tiny for an ordinary type-II superconductor. However for those particular ultraclean materials with very high H_{c2} and very small ε_F , where dHvA effect in the superconducting mixed state have been observed (see introduction), the value of $\sqrt{\mu/\omega_{c2}}$ is of the order of ten and the theory presented here has noticable region of applicability below the upper critical field.

As the final remarque, we have to remember that μ is the chemical potential less the energy band ε_b so that the limit (51) is different for different bands and less restrictive for the bands with smallest value of $\mu - \varepsilon_b \approx \varepsilon_F - \varepsilon_b$.

5 Conclusion

The grand canonical ensemble theory of de Haas-van Alphen effect in the normal and superconducting states of 2D and quasi 2D metals valid at $\mu \gg \omega_c$ is developed taking into consideration finite temperature, level broadening due to impurity scattering, spin paramagnetic splitting and additional suppression due to inhomogeneous order parameter distribution in the mixed state. The main results are represented by the expressions (23), (34) and (52), (53), (54) for the magnetization amplitude oscillations.

The straightforward generalization to the multiband case is obtained by the summation of these expressions over several energetic bands.

The limits of observation of dHvA effect near the upper critical field (51) in the superconducting mixed state will be of course different for different energetic bands being less restrictive for the bands with smallest orbit area ~ $(\varepsilon_F - \varepsilon_b)$.

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Appendix A : Calculation of α

In this Appendix, we perform the calculation of the coefficient $\alpha(H,T)$ in the quasi-classical limit. Effects of quantization on the upper critical field have already been studied by Gruenberg and Gunther (1968) for a 3D system. These authors give a method for the calculation of the corrections in the linearized gap equation, which can be adapted to our 2D case. According to equation (36) we have

$$\alpha(H,T) = \frac{1}{g} - T \sum_{\nu=0}^{+\infty} \bar{S}_{\tilde{\omega}_{\nu}}$$
(56)

where

$$\bar{S}_{\tilde{\omega}_{\nu}} = 2\Re \int e^{-\frac{H\rho^2}{2}} \tilde{G}^{\sigma}(\mathbf{R}, \tilde{\omega}_{\nu}) \tilde{G}^{-\sigma}(\mathbf{R}, -\tilde{\omega}_{\nu}) d\mathbf{R}.$$
(57)

In the 2D case, the Green's function $\tilde{G}^{\sigma}(\mathbf{R}, \tilde{\omega}_{\nu})$ in the representation \mathbf{R} , after the integration over orbit centers (Dworin 1966), is expressed as

$$\tilde{G}^{\sigma}(\mathbf{R},\tilde{\omega}_{\nu}) = N_0 \omega_c e^{-t/2} \sum_{r=0}^{+\infty} \frac{L_r(t)}{i\tilde{\omega}_{\nu} - \xi_r + \sigma \mu_e H}$$
(58)

where $L_r(t)$ is the Laguerre's polynomial of order $r, t = H\rho^2/2$, and

$$\xi_r = (r + \frac{1}{2})\omega_c - \mu.$$

Using the relation between Laguerre's polynomials

$$\int_0^{+\infty} e^{-2t} L_n(t) L_m(t) \, dt = \left(\frac{1}{2}\right)^{n+m+1} \frac{(m+n)!}{m! \, n!}$$

we obtain

$$\bar{S}_{\tilde{\omega}_{\nu}} = N_0 \omega_c \Re \sum_{r,l=0}^{+\infty} \frac{(r+l)!}{r! \, l!} \frac{(1/2)^{r+l}}{(i\tilde{\omega}_{\nu} + \xi_r - \mu_e H)(-i\tilde{\omega}_{\nu} + \xi_l + \mu_e H)}.$$
(59)

Following Gruenberg and Gunther (1968), we do the Gaussian approximation

$$\left(\frac{1}{2}\right)^{r+l} \frac{(r+l)!}{r!\,l!} \approx \frac{e^{-(r-l)^2/4r}}{(\pi r)^{1/2}}$$

valid for $\mu/\omega_c \gg 1$. Then we make use of the Poisson's formula which gives us three kinds of terms :

$$\bar{S}_{\tilde{\omega}_{\nu}} = \sum_{n,m=-\infty}^{+\infty} S^{nm}_{\tilde{\omega}_{\nu}},\tag{60}$$

$$S_{\tilde{\omega}_{\nu}}^{nm} \approx (-1)^{n+m} N_0 \omega_c \Re \int_0^\infty \int_0^\infty dy \frac{1}{\sqrt{\pi x}} \frac{e^{2\pi i (nx-my) - (x-y)^2/4x} \, dx \, dy}{(i\tilde{\omega}_{\nu} + \xi_x - \mu_e H)(-i\tilde{\omega}_{\nu} + \xi_y + \mu_e H)} \tag{61}$$

with

$$\xi_x = x\omega_c - \mu.$$

In the first term obtained for n = m = 0, we transform from integration over x and y to integration over the coordinates of the two-dimensional vectors **q** and **q'**, so that $\omega_c x = q^2/2m$, $\omega_c y = q'^2/2m$. Since **q** and **q'** are very close (and of order of k_F), we have

$$(x-y)^2/4x \approx (q-q')^2/2H$$

After using the following approximative relation

$$\frac{e^{-(q-q')^2/2H}}{\sqrt{qq'/2H}} \approx \frac{1}{\sqrt{\pi}} \int_0^{2\pi} e^{-(\mathbf{q}-\mathbf{q}')^2/2H} \, d\theta_{\mathbf{q}\mathbf{q}'}$$

changing variable \mathbf{q}' to $\mathbf{Q} = \mathbf{q} - \mathbf{q}'$ and neglecting the term $Q^2/2m$ in the energy $\xi_{q'}$, we obtain

$$S_{\tilde{\omega}_{\nu}}^{00} \approx \frac{N_0 \omega_c}{2\pi^2 H^2} \Re \int d\mathbf{Q} \, e^{-Q^2/2H} \int \frac{d\mathbf{q}}{(i\tilde{\omega}_{\nu} + \xi_q - \mu_e H)(-i\tilde{\omega}_{\nu} + \xi_q + \mu_e H - \mathbf{Q} \cdot \frac{\mathbf{q}}{m})}.$$
 (62)

Since q is very close to k_F , the term q/m is approximate by the Fermi velocity v_F . The integration over **q** is changed to an integral over energy and angle θ . The first integration over energy gives

$$S^{00}_{\tilde{\omega}_{\nu}} = \frac{N_0}{\pi H} \Re \int d\mathbf{Q} \, e^{-Q^2/2H} \int_0^{2\pi} \frac{d\theta}{2\tilde{\omega}_{\nu} + 2i\mu_e H - iv_F Q \cos\theta}.$$
 (63)

The second integration over the angle is performed by introducing the complex variable $z = e^{i\theta}$. The corresponding contour is the unity circle. We find

$$S_{\tilde{\omega}_{\nu}}^{00} = \frac{2N_0}{H} \Re \int \frac{e^{-Q^2/2H} \, d\mathbf{Q}}{\sqrt{(v_F Q)^2 + 4(\tilde{\omega}_{\nu} + i\mu_e H)^2}}.$$
 (64)

Rewriting this expression as

$$S^{00}_{\bar{\omega}_{\nu}} = 2\pi N_0 \zeta \Re \int_0^{+\infty} \frac{e^{-\zeta x} \, dx}{\sqrt{\kappa + x}} \tag{65}$$

where $\zeta = 1/\varepsilon_F \omega_c$ (ε_F is the Fermi level) and $\kappa = (\tilde{\omega}_{\nu} + i\mu_e H)^2$, then we calculate

$$S^{00} = \frac{T}{N_0} \sum_{\nu=0}^{+\infty} S^{00}_{\tilde{\omega}_{\nu}}$$

Using the following relation valid at low temperatures

$$2\pi T \sum_{\nu} F(\omega_{\nu}) = \int_{0}^{+\infty} F(\omega) \, d\omega + \frac{\pi^2}{6} T^2 \left(\frac{\partial F}{\partial \omega}\right)_{\omega=0} \tag{66}$$

we get

$$\frac{1}{gN_0} - S^{00} = \frac{\zeta}{2} \int_0^{+\infty} \ln x \, e^{-\zeta x} \, dx + \frac{\pi^2}{6} T^2 \zeta \sqrt{\kappa_0} \int_0^{+\infty} \frac{e^{-\zeta x} \, dx}{(x+\kappa_0)^{3/2}} - \ln \frac{\pi T_c}{\gamma}.$$
 (67)

Here $\kappa_0 = \Gamma + i\mu_e H$. In the first term in the right-hand side of equation (66), we neglect Γ and $\mu_e H$. To avoid the divergence, a cut-off ω_0 is introduced ; this latter vanishes with subtraction of the term $\frac{1}{N_{0g}} = \ln(\frac{2\gamma\omega_0}{\pi T_c})$ where $C = \ln \gamma$ is the Euler constant. Taking notes of the value of the integrals (Gradshteyn and Ryzhik 1980) :

$$\zeta \int_0^{+\infty} \ln x \, e^{-\zeta x} \, dx = -C - \ln \zeta$$

and

$$\frac{e^{-\zeta x} \, dx}{(x+\kappa_0)^{3/2}} = \frac{2}{\sqrt{\kappa_0}} - 2\sqrt{\pi\zeta} e^{\kappa_0 \zeta} \left(1 - \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{\zeta\kappa}} e^{-t^2} \, dt\right) \approx \frac{2}{\sqrt{\kappa_0}}$$

we obtain

$$\frac{1}{g} - T \sum_{\nu=0}^{+\infty} S_{\tilde{\omega}_{\nu}}^{00} = \frac{N_0}{2} \left\{ \ln(\frac{H}{H_{c2o}}) + \frac{2\pi^2}{3} \frac{T^2}{\mu\omega_c} \right\}$$
(68)

with $H_{c2o} = \frac{2\pi^2 T_c^2}{\gamma v_F^2}$. The temperature dependent term is neglected further in so far as we work at very low-temperatures.

For the second term obtained for $n = m \neq 0$ in (60), we follow the steps leading to equation (65). We approximate the additional term in the exponent by $2i\pi n(x-y) \approx 2i\pi nv_F \cos\theta$. Thus we find for n > 0, $S_{\omega_\nu}^{nn} = 0$ and for n < 0

$$S_{\tilde{\omega}_{\nu}}^{nn} = 2\pi N_0 \zeta \Re e^{-4\pi |n| \frac{(\tilde{\omega}_{\nu} + i\mu_e H)}{\omega_c}} \int_0^{+\infty} \frac{e^{-\zeta x} \, dx}{\sqrt{\kappa + x}}.$$
 (69)

Using the value of the integral (Gradshteyn and Ryzhik 1980)

$$\int_0^{+\infty} \frac{e^{-\zeta x} \, dx}{\sqrt{\kappa + x}} = \sqrt{\frac{\pi}{\zeta}} \, e^{\zeta \kappa} \left(1 - \frac{2}{\sqrt{\pi}} \int_0^{\sqrt{\zeta \kappa}} e^{-t^2} \, dt \right) \approx \sqrt{\frac{\pi}{\zeta}}$$

for $\zeta \kappa \ll 1$, we get

$$S_{\tilde{\omega}\nu}^{nn} = \frac{2\pi^{3/2}N_0}{\sqrt{\mu\omega_c}} \Re e^{-4\pi n \frac{(\tilde{\omega}\nu + i\mu_e H)}{\omega_c}}.$$
(70)

The third and last term in (60) containing the summation over $n \neq m$ is evaluated only for nonzero values of n and m because $S^{n0}_{\tilde{\omega}_{\nu}}$ and $S^{0n}_{\tilde{\omega}_{\nu}}$ are negligibly small. We approximate $(\pi x)^{-1/2} \exp[-(x-y)^2/4x]$ by $(\omega_c/\pi\mu)^{1/2}$ in order to have two uncoupled integrations. These are nonzero only for n and m negative and yield for a pair (n,m)

$$S_{\tilde{\omega}_{\nu}}^{nm} + S_{\tilde{\omega}_{\nu}}^{mn} = (-1)^{n+m} \frac{8\pi^{3/2} N_0}{\sqrt{\mu\omega_c}} \Re e^{-2\pi |n+m|(\frac{\tilde{\omega}_{\nu}+i\mu_e H}{\omega_c})} \cos(2\pi (n-m)\frac{\mu}{\omega_c}).$$
(71)

Reassembling all these different contributions, we have

$$\alpha(H,T) = \frac{N_0}{2} \left\{ \frac{H - H_{c2o}}{H_{c2o}} + \left(\frac{T}{T_c}\right)^2 S_0 - 2\sqrt{\pi} \sqrt{\frac{\omega_c}{\mu}} S_1 - 8\sqrt{\pi} \sqrt{\frac{\omega_c}{\mu}} S_2 \right\}$$
(72)

where

$$S_0 = \frac{2\pi^2 T_c^2}{3\mu\omega_c},\tag{73}$$

$$S_1 = \frac{2\pi T}{\omega_c} \Re \sum_{n=1}^{+\infty} \sum_{\nu=0}^{+\infty} e^{-4\pi n \left(\frac{\tilde{\omega}_\nu + i\mu_e H}{\omega_c}\right)},\tag{74}$$

$$S_2 = \frac{2\pi T}{\omega_c} \Re \sum_{n=1}^{+\infty} \sum_{m>n}^{+\infty} \sum_{\nu=0}^{+\infty} (-1)^{n+m} \cos(2\pi (n-m)\frac{\mu}{\omega_c}) e^{-2\pi (n+m)(\frac{\tilde{\omega}_{\nu}+i\mu_e H}{\omega_c})}.$$
 (75)

The term S_1 is the same as in the 3D case (Mineev 2000). We also do the same transformation and include it in the upper critical field at low temperatures averaged over the oscillations. Like in (Mineev 2000), we simplify the term S_2 in (75) changing summation variables to nand m - n = l, and keeping reasonably only the first term in the sum over n

$$S_2 = \frac{\pi T}{\omega_c} \sum_{l=1}^{+\infty} (-1)^l \frac{e^{-2\pi(l+2)\frac{\Gamma}{\omega_c}}}{\sinh \lambda_{l+2}} \cos(2\pi(l+2)\frac{\mu_e H}{\omega_c}) \cos(2\pi l\frac{\mu}{\omega_c}).$$
(76)

This is the term which is taken into account in α_{osc} .

In the quasi 2D case, we can follow exactly the same previous proceeding to calculate the coefficient α . The Green's function is expressed in a mixt representation (x, y, k_z)

$$\tilde{G}^{\sigma}(x, y, k_z, \tilde{\omega}_{\nu}) = N_0 \omega_c e^{-t/2} \sum_{r=0}^{+\infty} \frac{L_r(t)}{i\tilde{\omega}_{\nu} - (r + \frac{1}{2})\omega_c + 2t\cos(k_z d) + \mu + \sigma\mu_e H}.$$
(77)

In equation (57), in addition to the integration over the two-dimensional vector \mathbf{R} there is an additional k_z integration. At last, we obtain

$$\alpha^{q2d}(H,T) = \frac{N_0}{2d} \left\{ \frac{H - H_{c2o}}{H_{c2o}} + \left(\frac{T}{T_c}\right)^2 S_0 - 2\sqrt{\pi}\sqrt{\frac{\omega_c}{\mu}} S_1 - 8\sqrt{\pi}\sqrt{\frac{\omega_c}{\mu}} S_2 \right\}$$
(78)

where

$$\begin{split} S_0^{q2d} &= \frac{S_0^{2d}}{d}, \\ S_1^{q2d} &= \frac{S_1^{2d}}{d}, \\ S_2^{q2d} &= \frac{\pi T}{\omega_c} \sum_{l=1}^{+\infty} (-1)^l \frac{e^{-2\pi (l+2)\frac{\Gamma}{\omega_c}}}{\sinh \lambda_{l+2}} \cos(2\pi (l+2)\frac{\mu_e H}{\omega_c}) J_0(2\pi l\frac{2t}{\omega_c}) \cos(2\pi l\frac{\mu}{\omega_c}). \end{split}$$

Therefore, the oscillating part of α includes an additional Bessel function factor analogous to that in quasi 2D normal metal expressions.

Appendix B : Calculation of β

The calculation of the coefficient β is performed in the magnetic sublattices' representation (Vavilov and Mineev 1997)

$$\beta(H,T) = \frac{T}{2} \sum_{\sigma \pm 1} \sum_{\nu} \sum_{n,n',m,m'} G^{-\sigma}(\xi_n, -\tilde{\omega}_\nu) G^{\sigma}(\xi_m, \tilde{\omega}_\nu) G^{-\sigma}(\xi_{n'}, -\tilde{\omega}_\nu) \times G^{\sigma}(\xi_{m'}, \tilde{\omega}_\nu) F_{mm'}^{nn'}$$
(79)

where $F_{mm'}^{nn'} = \int \frac{d\mathbf{q}}{(2\pi)^2} f_{nm}(\mathbf{q}) f_{nm'}^*(\mathbf{q}) f_{n'm}(\mathbf{q}) f_{n'm'}^*(\mathbf{q})$ are the matrix elements of the Abrikosov's function f. Keeping only the main contribution to the expression (79) given by the diagonal terms n = n' = m = m', and since $F_{nn}^{nn} \approx H/(2\pi)^2 n$ (Vavilov and Mineev 1997), we have

$$\beta(H,T) = \frac{H}{2(2\pi)^2} \sum_{\sigma \pm 1} T \sum_{\nu} \sum_{n=0}^{+\infty} \frac{[G^{\sigma}(\xi_n, \tilde{\omega}_{\nu})G^{-\sigma}(\xi_n, -\tilde{\omega}_{\nu})]^2}{n}.$$
 (80)

The use of the Poisson's summation formula to transform the summation over n leads to a smooth non-oscillating field dependent part and to a fast oscillating field dependent part of β . The smooth part is obtained by the substitution of the summation by the integration with

$$\frac{H}{2\pi} \sum_{n=0}^{+\infty} = \frac{H}{2\pi} \int_{n=0}^{+\infty} = N_0 \int d\xi$$

and $n \approx \mu/\omega_c$:

$$\bar{\beta}(H,T) = \frac{N_0\omega_c}{4\pi\mu} \sum_{\sigma\pm 1} T \sum_v \int_{-\infty}^{+\infty} \frac{d\xi}{[(i\tilde{\omega}_\nu - \xi + \sigma\mu_e H)(-i\tilde{\omega}_\nu - \xi - \sigma\mu_e H)]^2}.$$
 (81)

The integration over energy ξ gives

$$\bar{\beta}(H,T) = N_0 \frac{\omega_c}{4\mu} T \sum_{\nu=0}^{+\infty} \frac{\tilde{\omega}_{\nu}^3 - 3\tilde{\omega}_{\nu}(\mu_e H)^2}{(\tilde{\omega}_{\nu}^2 + (\mu_e H)^2)^2}.$$
(82)

This expression is then performed at T = 0 K to allow the change of the summation to the integration. We find

$$\bar{\beta}(H,0) = N_0 \frac{\omega_c}{16\pi\mu} \frac{\Gamma^2 - (\mu_e H)^2}{(\Gamma^2 + (\mu_e H)^2)^2}.$$
(83)

The oscillating part of $\beta(H,T)$ is given by

$$\beta_{osc}(H,T) = \frac{N_0 \omega_c}{2\pi\mu} \Re \sum_{\sigma \pm 1} T \sum_{\nu} \sum_{l=1}^{+\infty} (-1)^l e^{2\pi i l \frac{\mu}{\omega_c}}$$
$$\times \int_{-\infty}^{+\infty} \frac{e^{-2\pi i l \frac{\xi}{\omega_c}} d\xi}{(i\tilde{\omega}_{\nu} - \xi + \sigma\mu_e H)^2 (-i\tilde{\omega}_{\nu} - \xi - \sigma\mu_e H)^2}.$$
(84)

The integration over ξ presents no difficulty

$$\beta_{osc}(H,T) = \frac{N_0 \omega_c}{\mu} \sum_{l=1}^{+\infty} (-1)^l \cos(2\pi l \frac{\mu}{\omega_c}) \Re T \sum_{\nu=0}^{+\infty} e^{-2\pi l (\frac{\tilde{\omega}_\nu + i\mu_e H}{\omega_c})} \times \left\{ \frac{1}{(\tilde{\omega}_\nu + i\mu_e H)^3} + \frac{2\pi l}{\omega_c (\tilde{\omega}_\nu + i\mu_e H)^2} \right\}.$$
(85)

At T = 0, the summation over ν is replaced by the integration, which yields at last

$$\beta_{osc}^{2d}(H,T=0) = \frac{N_0\omega_c}{2\pi\mu\Gamma^2} \sum_{l=1}^{+\infty} (-1)^l \cos(2\pi l \frac{\mu}{\omega_c}) I(2\pi l \frac{\Gamma}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}}$$
(86)

where

$$I(x) = \int_0^\infty \left[\frac{1}{(y+1)^3} + \frac{x}{(1+y)^2}\right] e^{-xy} \, dy.$$

m the same calculations yields

For a quasi 2D system, the same calculations yields

$$\bar{\beta}^{q2d}(H,0) = \frac{\bar{\beta}^{2d}(H,0)}{d} \tag{87}$$

and like in the oscillating part of α , an additional Bessel's function factor appears the oscillating part of β

$$\beta_{osc}^{q2d}(H,0) = \frac{N_0}{d} \frac{\omega_c}{2\pi\mu\Gamma^2} \sum_{l=1}^{+\infty} (-1)^l \cos(2\pi l \frac{\mu}{\omega_c}) I(2\pi l \frac{\Gamma}{\omega_c}) J_0(2\pi l \frac{2t}{\omega_c}) e^{-2\pi l \frac{\Gamma}{\omega_c}}.$$
 (88)

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