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de Haas–van Alphen oscillations in high-temperature superconductors

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Recent de Haas–van Alphen (dHvA) experiments on high-T_c compounds have been interpreted using Lifshitz-Kosevich (LK) theory, which ignores many-body effects. However in quasi-2d systems, interactions plus Landau-level quantization give strong singularities in the self-energy Σ and the thermodynamic potential Ω. These are rapidly suppressed as one increases the c-axis tunneling amplitude $t_\perp$ and/or impurity scattering. We show that interaction effects should show up in these experiments, and that they can lead to strong deviations from LK behavior. Moreover, dHvA experiments in quasi-2d systems should clearly distinguish between Fermi-liquid and non-Fermi-liquid states, for sufficiently weak impurity scattering.

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By tradition de Haas–van Alphen (dHvA) experiments are interpreted using Lifshitz-Kosevich (LK) theory, in which magnetization oscillations probe directly the quasiparticles at the Fermi surface (so that in a non-Fermi liquid (NFL), with zero quasiparticle weight on this surface, LK theory implies no dHvA oscillations at all). Where applicable, LK theory allows unambiguous measurement of Fermi-surface cross-sectional areas, Fermi-surface scattering rates, and Fermi-surface band masses.[1]

Even in three dimensions (3d), LK theory is not strictly valid because of interactions;[2,3] these cause "Engelsberg-Simpson" (ES) deviations from LK, which are seen in experiments.[4] In two dimensions (2d), the mere existence of the fractional quantum Hall liquid (FQHL), even when the interaction strength $\bar{V} \ll \hbar\omega_c$, shows that Fermi-liquid (FL) theory must break down in a field, provided impurity scattering is weak[5] (i.e., once $\omega_c\tau \gg 1$, where ω_c is the cyclotron frequency and τ an impurity scattering time).

Thus the dHvA experiments recently performed in high-T_c systems[6] create a clear paradox. Impurity scattering is weak (it must be for a dHvA signal to be seen) and the c-axis tunneling amplitude $t_\perp$ is argued to be very small (in $YBa_2Cu_3O_{6.5}$ (YBCO), $t_\perp \sim 15$ K is claimed), implying that $\hbar\omega_c > t_\perp$ and the system is reaching the 2d limit. And yet it is also claimed that the data can be fit using LK theory.[6] Similar LK analyses have been made for other quasi-2d systems.[7,8] Since LK theory must break down for genuinely 2d systems if $\omega_c\tau \gg 1$ and correlations are strong, this raises several important questions:

(a) how can one generalize dHvA theory to include interactions in quasi-2d systems, and how should dHvA data then be analyzed;

(b) what kind of oscillations will be shown by NFL systems, and can one tell the difference between FL and NFL states from dHvA experiments?

To address these questions, we first analyze the one-particle Green's function $\mathcal{G}$ and the thermodynamic potential Ω for a quasi-2d system, with $t_\perp/\hbar\omega_c$ assumed arbitrary (but $t_\perp \ll \mu$, the chemical potential). We find that interactions give highly singular behavior in $\mathcal{G}$, which when $t_\perp \ll \hbar\omega_c$ and $\omega_c\tau \gg 1$ causes a complete breakdown of standard Fermi-liquid theory. However we still find dHvA oscillations, although not of LK form. To illustrate these results we compute $\mathcal{G}$ for two examples: a NFL with singular forward-scattering interactions, and a FL of band electrons interacting with nearly antiferromagnetic spin fluctuations. We find clear departures from LK behavior, whose form depends strongly on the nature of the many-body interactions; thus dHvA experiments ought to be able to distinguish FL from NFL states. Neither LK theory nor its "ES" generalisation,[3] apply strictly unless $\hbar\omega_c < t_\perp$ and/or $\omega_c\tau \ll 1$.

(i) Singularities of $\mathcal{G}$: the form of the dHvA oscillations can be found from either $\mathcal{I}m\mathcal{G}(\epsilon)$, or directly from Ω. In noninteracting 2d systems, the Landau levels are massively degenerate, and $\mathcal{I}m\mathcal{G}_\nu(\epsilon) \propto \delta(\epsilon-\epsilon_\nu)$, where ϵ_ν is the νth Landau-level energy. Interactions destabilize this degeneracy, and so have a singular effect on $\mathcal{G}(\epsilon)$. However any impurity scattering or c-axis tunneling tends to suppress this singularity. Although the analytic structures of $\mathcal{G}(\epsilon)$ and Ω are now understood for *neutral* 2d fermions[9] in a field (i.e., without Landau quantization), there are no general results when one has both Landau quantization and interactions.[10] However, we can derive results for particular models; here we study quasi-2d band electrons, with dispersion $\epsilon_{\mathbf{k}} = \varepsilon(k_x,k_y) - 2t_\perp\cos(k_z a) - \mu$, where $t_\perp \ll \mu$, coupled to low-energy fluctuations. In a finite field, the lowest-order "one-fluctuation" graph for the self-energy then takes the form

$$\Sigma_\nu(k_z,z) = \sum_{\mathbf{q}}\sum_{\nu'}\int \frac{d\omega}{\pi}|\Lambda_{\nu\nu'}(\mathbf{q})|^2 \mathcal{I}m\chi(\mathbf{q},\omega) \times\left(\frac{1-f_{\nu'}+n(\omega)}{z-\omega-\epsilon_{\nu'}(q_z)} + \frac{f_{\nu'}+n(\omega)}{z+\omega-\epsilon_{\nu'}(q_z)}\right) \quad (1)$$

where z is a complex frequency, $\chi(\mathbf{q},\omega)$ is the fluctuation propagator, $f_\nu = f(\epsilon_{\nu q_z})$ is the Fermi function for electrons in the νth Landau level, $n(\omega)$ the Bose function, and the matrix element $\Lambda_{\nu\nu'}(\mathbf{q})$, between Landau states ν,ν' and the fluctuations, incorporates the fermion-fluctuation coupling g_q. When $\mu \gg \omega_c$, $|\Lambda_{\nu\nu'}(\mathbf{q})|^2 \sim g_q^2(m/2\mu)^{1/2}\omega_c/\pi q$. Quite generally the self-energy for a quasi-2d system can be written near the Fermi surface as $\Sigma(z) = \bar{\Sigma}(z) + \Sigma_{osc}(z)$, where $\bar{\Sigma}(z)$ is nonoscillatory in $1/B$, and the oscillatory part

$$\Sigma_{osc}(z) = 2\sum_{r=1}^{\infty}(-1)^r\Sigma_r(z)J_0\left(4\pi r\frac{t_\perp}{\hbar\omega_c}\right)\sin\left(2\pi r\frac{A_F}{B}\right). \quad (2)$$

The Bessel function J_0 in this expression comes from integrating over q_z.

To illustrate how Landau quantization affects the self-energy, we begin by analyzing two widely studied models of strong correlations in quasi-2d systems: in zero field these describe a FL and NFL, respectively.

Model (a) spin fluctuation model: this well-known model[11] has 2d lattice fermions with dispersion

$$\varepsilon(k_x,k_y) = -2t_0(\cos k_x + \cos k_y) - 4t_1 \cos k_x \cos k_y \quad (3)$$

and coupling $t_\perp$ between planes; the fermions couple to antiferromagnetic spin fluctuations, with propagator

$$\chi(\mathbf{q},\omega) = \frac{\chi_0}{1+\xi^2(\mathbf{q}-\mathbf{Q})^2 - i\omega/\omega_{SF}} \quad (4)$$

via a coupling $g_q=g$. The wave vectors $\mathbf{Q}=(\pm\pi,\pm\pi)$. In zero field this model, with or without vertex corrections,[12] gives FL behavior: the Green's function has finite Fermi-surface residue $z_{k_F}(\mu)$, and the self-energy has a 2d FL form, with $\mathcal{R}e\Sigma(\omega)=(1-m/m^*)\omega$ and $\mathcal{I}m\Sigma(\omega)\propto\omega^2(1+\ln\omega)$.

In a finite field, the one-fluctuation form (1) for $\Sigma(\omega)$ can be evaluated analytically.[13] The essential result is shown in Fig. 1; Landau quantization introduces a "steplike" behavior in $\partial\mathcal{I}m\Sigma/\partial\epsilon$, with corresponding singularities in $\mathcal{R}e\Sigma(\epsilon)$, at $\epsilon=\epsilon_\nu$. Notice how rapidly this singular behavior is suppressed by interplane hopping—it is almost invisible once $t_\perp\sim\hbar\omega_c$. Impurity scattering has a similar effect (not shown in Fig. 1).

Model (b) non-Fermi-liquid model: we now couple the band electrons to fluctuations with propagator,[14]

$$\chi(\mathbf{q},\omega) = \frac{q}{\chi q^s - i\gamma\omega} \quad (5)$$

where s is a dynamic scaling exponent, with $2\leq s\leq 3$, using a fermion-fluctuation coupling $g_q=K_s$. The zero-field self-energy has the NFL forms $\Sigma(\epsilon)\sim\epsilon\ln\epsilon$ (for $s=2$) and $\Sigma(\epsilon)\sim(i\Omega_0/\epsilon)^{1/3}\epsilon$ (for $s=3$) so that $z_{\mathbf{k}}(\epsilon)\to 0$ on the Fermi surface.[14] In finite field, the one-fluctuation self-energy (1) can be found analytically, in the form (2); the $T=0$ coefficients $\Sigma_r(z)$ are found to be

$$\Sigma_r(z) = \frac{sK_s}{2r^{2/s}}\left[\mathcal{Z}_r^{1/2}S_2\left(\frac{1}{2}+\frac{2}{s},\frac{1}{2};\mathcal{Z}_r\right) - \mathcal{Z}_r^{2/s} - (-\mathcal{Z}_r)^{1/2}S_2\left(\frac{1}{2}+\frac{2}{s},\frac{1}{2};-\mathcal{Z}_r\right) + (-\mathcal{Z}_r)^{2/s}\right] \quad (6)$$

with a more complicated finite T form. Here S_2 is a Lommel function,[15] and $\mathcal{Z}_r=2\pi rz/\hbar\omega_c$. Now the singular behavior in Σ is far more pronounced; again, it is eliminated by switching on $t_\perp$ [Fig. 1(b)], or by impurity scattering [calculated in Fig. 1(c) in a self-consistent Born approximation].

We see that both models show singular behavior of $\Sigma(\epsilon)$ as a function of ϵ, implying similar behavior for the quasi-

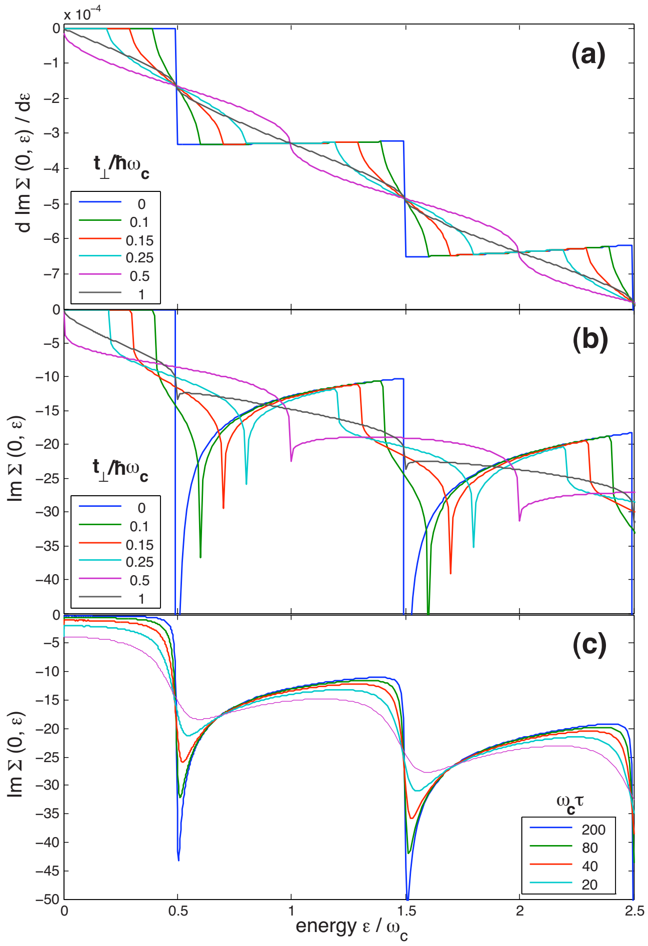

FIG. 1. (Color online) The imaginary part $\mathcal{I}m\Sigma(\epsilon)$ of the self-energy, as a function of $t_\perp/\hbar\omega_c$, at $T=0$. (a) shows $\mathcal{I}m\,\partial\Sigma/\partial\epsilon$ for the spin-fluctuation model; we fix $g_q=g=0.58$ eV, $\chi_0=80$ states/eV, $\xi=2.5a$, and $\omega_{SF}=10$ meV. (b) shows $\mathcal{I}m\Sigma$ (with no derivative) for the non-Fermi-liquid model, assuming $s=3$; we fix $K_{s=3}=0.013(\hbar\omega_c)^{2/3}\mu^{1/3}$ with $\mu=6000$ K. (c) shows the effect of impurity scattering on the NFL model; we plot $\mathcal{I}m\Sigma(\epsilon)$ for different values of $\omega_c\tau$, assuming $t_\perp/\hbar\omega_c=0.75$.

particle weight $z_k(\epsilon)$; we expect this behavior to survive vertex corrections.[12] At the Fermi energy, $\Sigma(\epsilon=\mu)$ will then show the same singular behavior as a function of B, periodic in $1/B$. Strictly speaking, this means a breakdown of FL theory for both models, but much more strongly for the NFL system. Because these singularities are rapidly suppressed by both interplane hopping and impurity scattering, this breakdown will only be clearly visible when $t_\perp,\hbar/\tau\ll\hbar\omega_c$.

(ii) Thermodynamic potential Ω: let us now consider the two questions posed in the introduction, by considering $\Omega(B)$ to all orders in fluctuation graphs. If "crossed graphs" can be ignored in $\Sigma(z)$, we can write an expression for Ω in terms of $\mathcal{G}$,[16]

$$\Omega = -\frac{1}{\beta}\mathrm{Tr}\ln[(\overline{\mathcal{G}}+\mathcal{G}_{osc})^{-1}] \quad (7)$$

where $\overline{\mathcal{G}}$ is the nonoscillatory part of $\mathcal{G}$. This generalizes the classic Luttinger/ES result[3] for Ω, which drops $\mathcal{G}_{osc}$ from

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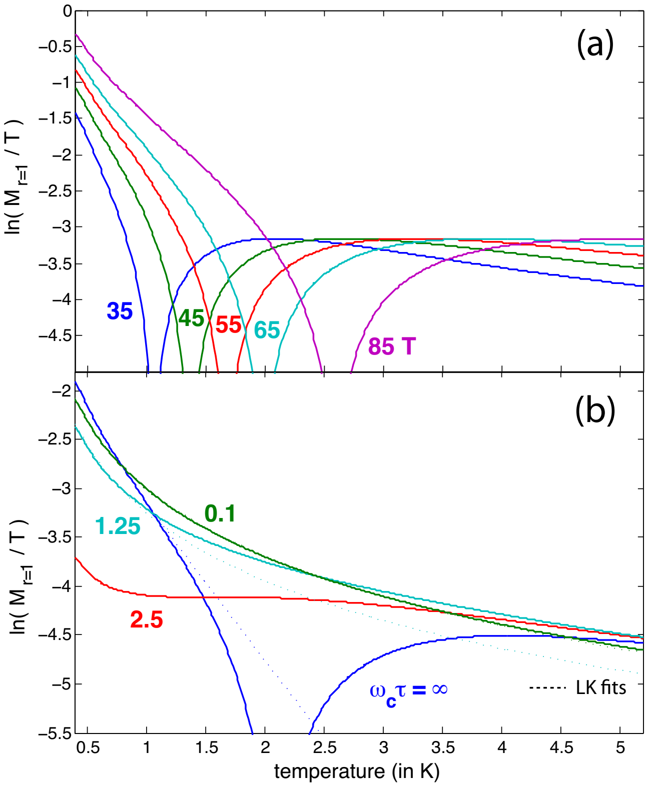

FIG. 2. (Color online) $\ln M_r/T$ for $r=1$ against T (the "mass plot"), for the spin-fluctuation model: (a) plot for different fields, assuming $t_\perp=15$ K but no impurity scattering (when $B=55$ T, $\hbar\omega_c=20$ K); (b) plot for different impurity scattering rates, assuming $t_\perp/\hbar\omega_c=0.6$. The dashed lines are fits to LK.

Eq. (7). This neglect is justified in 3d but not in 2d (Ref. 16); in the quasi-2d case it is only justified if $t_\perp \gg \hbar\omega_c$. From Eq. (7) we find $\Omega=\bar{\Omega}+2\Sigma_{r=1}^{\infty}(-1)^r(\Omega_1^r+\Omega_2^r)\cos(r\hbar A_F/eB)$, where $\bar{\Omega}$ is the nonoscillatory part of Ω, and

$$\Omega_1^r = \frac{m\omega_c kT}{2\pi r\hbar}\sum_{n>0} J_0\left(\frac{4\pi r t_\perp}{\hbar\omega_c}\right)e^{-2\pi r/\hbar\omega_c[\omega_n+\zeta(\omega_n)]}$$

$$\Omega_2^r = -\frac{mkT}{\hbar^2}\sum_{n>0} J_0\left(\frac{4\pi r t_\perp}{\hbar\omega_c}\right)\zeta_r(\omega_n) \quad (8)$$

where $\omega_n=(2n+1)\pi kT$, and $\zeta_r(\omega_n)=i\Sigma_r(i\omega_n)$ is real and positive. Equation (8) reduces to the Luttinger/ES expression for Ω if we drop Ω_2, and use only the nonoscillatory part $\bar{\zeta}(\omega_n)$ of $\zeta(\omega_n)=i\Sigma(i\omega_n)$ in Ω_1. However Fig. 1 shows that the oscillatory part of Σ must not in general be neglected. Ω_1 reduces to LK theory, including the J_0 term,[18] only if either $\Sigma(\omega)=0$, or $\Sigma(\omega)\to(1-m/m^*)\omega+i/2\tau$, i.e., a mass renormalization and scattering rate both independent of energy.

(iii) Oscillatory magnetization: we write the magnetization at constant chemical potential $M_\mu(B)=-\partial\Omega/\partial B|_\mu$ in the form $M=\bar{M}(B)+2\Sigma_r(-1)^r M_r$, where $\bar{M}$ is the nonoscillatory part [$M(B)$ at constant N is found by making a Legendre transform[17]]. Differentiating Eq. (8), we get $M_r=M_1^r+M_2^r$,[19] with

$$M_i^r(B,T) = \frac{\hbar r A_F}{eB^2}\Omega_i^r(B,T)\sin(r\hbar A_F/eB). \quad (9)$$

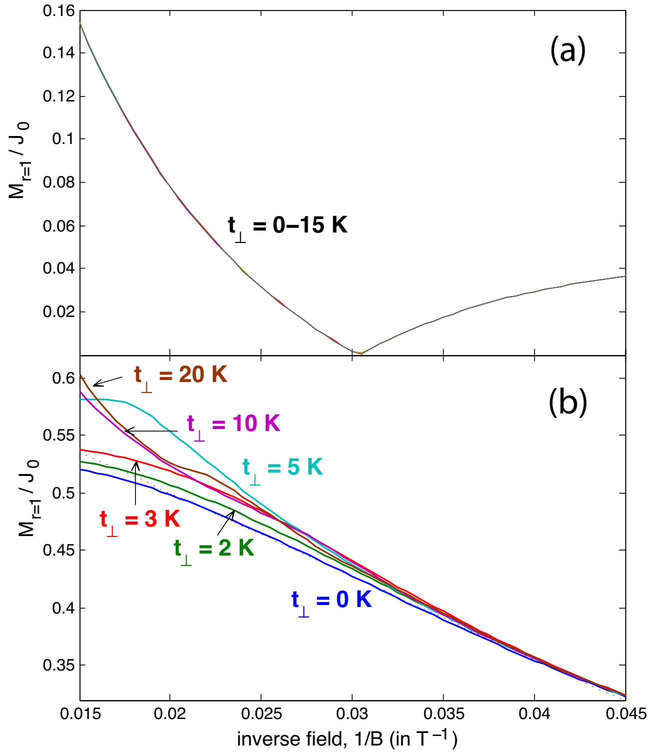

FIG. 3. (Color online) The dHvA component M_r/J_0 for $r=1$, against $1/B$ (again, if $B=55$ T, $\hbar\omega_c=20$ K), for different values of $t_\perp$ (measured in K), with no impurity scattering; we assume $T=1$ K. (a) for the spin-fluctuation model; (b) for the non-Fermi-liquid model with $s=3$. The dashed line is an example of an LK fit.

This result is strikingly different from LK and Luttinger/ES theory, with *two* oscillatory terms. Key features of Eq. (9) are:

(1) without interactions, or when $\partial\Sigma/\partial\omega$ is negligible, we get LK theory,

$$M_r^{LK} \propto \frac{kT}{\sinh\left(\frac{2\pi^2 rkT}{\hbar\omega_c}\right)}J_0\left(\frac{4\pi r t_\perp}{\hbar\omega_c}\right)\exp\left(-\frac{r}{\omega_c\tau}\right). \quad (10)$$

However interactions will give clear departures from LK theory, even in mass plots (Fig. 2), unless the fluctuation energy scale $\gg\hbar\omega_c$, and/or $\omega_c\tau<1$. Both M_1 and M_2 contribute to deviations from LK. However, the two terms compete: M_1^r is suppressed exponentially by self-energy corrections, whereas the new term M_2^r *increases* linearly with these. Thus interactions lead to strong departures from LK, and NFL have much stronger departures than FL. Thus dHvA experiments can test for departures from FL theory.

(2) The form of $M(B)$ depends strongly on $t_\perp/\hbar\omega_c$. This gives a remarkable structure in field plots (Fig. 3), which is eliminated by strong impurity scattering [Fig. 2(b)] or by removing strong correlation effects.

(3) Short-range impurity scattering strongly suppresses the singular structure from interactions once $\omega_c\tau<1$ [see Fig. 2(b)]. Again, M_1 and M_2 behave differently: M_1^r decreases exponentially with $1/\omega_c\tau$ (à la Dingle) but M_2^r decreases approximately as a power law.

Summarizing, we see that interactions have profound effects on the quasiparticles and the thermodynamics of conducting systems in high fields, for quasi-2d systems. These effects are rapidly removed by interplane coupling (once $t_\perp>\hbar\omega_c$), and even more rapidly by impurity scattering (once $\omega_c\tau<1$).

Consider now the experimental situation. At first glance, experiments on YBCO fall precisely in the crossover regime; $t_\perp\sim 15$ K is claimed,[6] and $15\lesssim\hbar\omega_c\lesssim 30$ K. However these results are misleading, because the fits (to LK theory) have not included the J_0 term in Eq. (10). Revised fits will certainly change the value of $t_\perp$, as well as the dHvA frequencies; they should include not only M_1^r but also M_2^r. It will be extremely interesting to fit data to different strong-correlation models, and discriminate between FL and NFL models. We note that a small or absent M_2^r term would suggest the underlying state is FL; a strong M_2^r term would indicate the system is NFL. It will also be interesting to look more closely at other strongly correlated quasi-2d systems in high fields. Finally, note that any other experiments, sensitive to the singular structure we find in $\mathcal{G}$, should show interesting effects. Obvious examples are c-axis tunneling and SdH experiments in very high fields, but a generalization to a transport theory will be required.

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[13] The self-energy $\Sigma(z)$, and the coefficients $\Sigma_r(z)$, can be found analytically for the spin-fluctuation model as a rather cumbersome function of elliptic integrals and exponential integrals.

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