Lifshitz transition with interactions in high magnetic fields

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(Received 16 January 2011; published 23 March 2011)

Motivated by a discontinuous transition observed in $CeIn_3$ in high magnetic fields, the effects of Landau quantization and interaction on a Lifshitz transition are studied. The Landau quantization leads to a quasi-one-dimensional behavior for the direction parallel to the field. Repulsive Coulomb interactions give rise to a gas of strongly coupled particles. The density correlation function is calculated for a special long-ranged potential. It is concluded that in the ground state, an electron pocket is emptied in a discontinuous fashion as a function of the chemical potential. This discontinuity is gradually smeared by the temperature, in agreement with the experiment.

DOI: 10.1103/PhysRevB.83.115133 PACS number(s): 71.27.+a, 71.70.Di, 71.10.Pm

I. INTRODUCTION

$CeIn_3$ is a cubic heavy fermion metal that orders antiferromagnetically with $T_N = 10.1$ K.[1] The Néel temperature is reduced with pressure and tends to zero at a critical pressure P_c of approximately 2.5 GPa. At P_c, the compound exhibits pressure-induced superconductivity with a maximum T_c of about 170 mK.[2] The superconducting dome is believed to be mediated by the antiferromagnetic fluctuations, which predominantly arise from "hot spots" on the Fermi surface.[3,4] This phase diagram consisting of an antiferromagnetic and a Kondo phase separated by a quantum critical point is consistent with the picture proposed by Doniach.[5]

The Néel ordered state is also suppressed as a function of magnetic field at $H_N = 61$ T at ambient pressure.[6] The Fermi surface cross sections above and below H_N differ, leading to the postulation that the transition is associated with a Fermi surface reconstruction with the $4f$ electrons being localized above H_N (small Fermi surface). This contrasts with the Fermi surface at high pressures ($P > P_c$) where the pockets found have a large Fermi surface,[6] since pressure increases the hybridization of the $4f$ electrons and renders states that are more itinerant in the paramagnetic phase.[7]

Small heavy f-carrier pockets located near the hot spots of antiferromagnetic fluctuations were observed within the Néel ordered phase.[6,8] These pockets collapse and become depopulated for fields larger than 41 T. Although there is insufficient experimental evidence to determine if the Lifshitz transition is caused by electron or hole pockets, in Refs. 6 and 8 the pockets are believed to be hole pockets. Harrison *et al.*[6] proposed that the disappearance of the pockets is associated with a Lifshitz transition.[9] Further studies of the H-P phase diagram[10] revealed that there are two transition lines for $CeIn_3$, i.e., one corresponding to the transition from the Néel state into the paramagnetic phase and a second transition line at lower magnetic fields caused by the reconstruction of the Fermi surface [see Fig. 1(a)]. The two lines merge at a pressure of about 2 GPa. The second transition, measured in the skin depth with a tunnel diode oscillator technique (TDO), displays hysteresis and becomes better defined at lower temperatures. Extrapolated to $T \to 0$, the transition represents a jump in the conductivity to a less resistive state at higher fields.

This discontinuous behavior is not compatible with a traditional Lifshitz transition, which leads to a gradual disappearance of a section of the Fermi surface and hence to a continuous change in the conductivity. Yamaji *et al.*[11] have shown that in two dimensions, the presence of interactions can turn the Lifshitz transitions discontinuous in contrast to the continuous transition for noninteracting systems. $CeIn_3$ is a three-dimensional system with strong correlations and the transition takes place in high magnetic field, so that the Landau quantization of the electron states plays an important role. We study the effects of the correlations on the density-density response function in the extreme quantum limit where only one Landau level is occupied. It is concluded that the system is strongly correlated and that the density correlation function diverges when the van Hove singularity of the empty band is approached. Consequently, the Lifshitz transition is transformed into a discontinuous transition, in agreement with the experimental observations. The discontinuity is gradually smeared by temperature.

The remainder of the paper is organized as follows. In Sec. II, we discuss the Lifshitz transition for a noninteracting system in a strong magnetic field, which leads to one-dimensional van Hove singularities. In Sec. III, we discuss the three-dimensional interacting gas of electrons with Landau quantization. In the leading logarithmic approximation, the parquet equations can be reduced to integro-differential equations.[12] The length scale in the screened Coulomb interaction prevents an exact analytic solution of these equations. However, by choosing an infinite-ranged potential in the plane perpendicular to the magnetic field,[13] the equations reduce to differential ones and the model can be solved via bosonization of fermions or the multiplicative renormalization group.[14] The system is strongly coupled and the strong-coupling fixed point has dramatic consequences for the Lifshitz transition. In Sec. IV, we calculate the density-density correlation function and conclude that the transition to the empty pocket has to be discontinuous. A brief summary is presented in Sec. V.

II. LIFSHITZ TRANSITION IN A STRONG MAGNETIC FIELD

We consider a small pocket of electrons in contact with an electron reservoir pinning the chemical potential. At this point, we neglect the interactions among the particles. For a

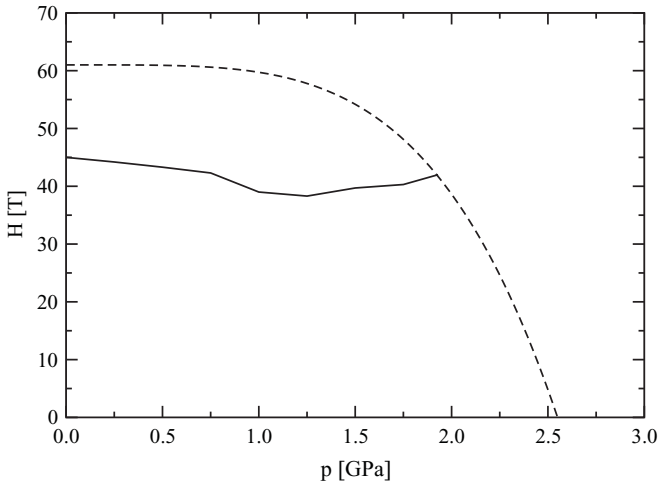

FIG. 1. Low-temperature magnetic field vs pressure phase diagram for $CeIn_3$ from Ref. 10. The dashed curve represents the Néel field destroying the antiferromagnetic long-range order. The solid line corresponds to the second transition line along which the Fermi surface reconstructs.

magnetic field pointing in the z direction, the energy levels of the states in the pocket are given by

$$\epsilon_\sigma(k_z,n) = \frac{\hbar^2 k_z^2}{2m} + 2\mu_B B\left(n+\frac{1}{2}\right) - \sigma g \mu_B B/2, \qquad (1)$$

where $\sigma = \pm 1$ and the g factor is assumed to be $10/7$ since the heavy electrons arise mostly from the Γ_7 states of the Ce $4f$ shell. Here $\mu_B = e\hbar/(2mc)$ and the degeneracy of the Landau level is $d = L_x L_y eB/(2\pi\hbar c)$, where $L_x L_y$ is the cross section of the sample perpendicular to the field. This dispersion leads to the following density of states (DOS) for up- and down-spins:

$$\rho_\uparrow(\omega) = \frac{eB\sqrt{2m}}{c(2\pi\hbar)^2}\sum_{n=0}^{\infty}[\omega-(2n+1-g/2)\mu_B B]^{-1/2},$$
$$\rho_\downarrow(\omega) = \frac{eB\sqrt{2m}}{c(2\pi\hbar)^2}\sum_{n=0}^{\infty}[\omega-(2n+1+g/2)\mu_B B]^{-1/2}. \qquad (2)$$

Note that the DOS for up-spins starts at $\omega = (1-g/2)\mu_B B$, while the one for down-spins begins at $(1+g/2)\mu_B B$. Each of the Landau levels contributes with a one-dimensional (energy minimum) van Hove singularity, which are displayed in Fig. 2(a) as a function of frequency. Due to the Zeeman splitting, the square-root singularities appear at different energies for up- and down-spin carriers. The physics of Lifshitz transitions in a strong magnetic field has been discussed by Blanter *et al.*[15]

At $T = 0$, the DOS is filled up to the chemical potential μ, which is pinned by the electron reservoir. The occupation for up-spin and down-spin electrons is given by

$$n_\uparrow(B) = 2\frac{eB\sqrt{2m}}{c(2\pi\hbar)^2}\sum_{n=0}^{\infty}[\mu-(2n+1-g/2)\mu_B B]^{1/2},$$
$$n_\downarrow(B) = 2\frac{eB\sqrt{2m}}{c(2\pi\hbar)^2}\sum_{n=0}^{\infty}[\mu-(2n+1+g/2)\mu_B B]^{1/2}. \qquad (3)$$

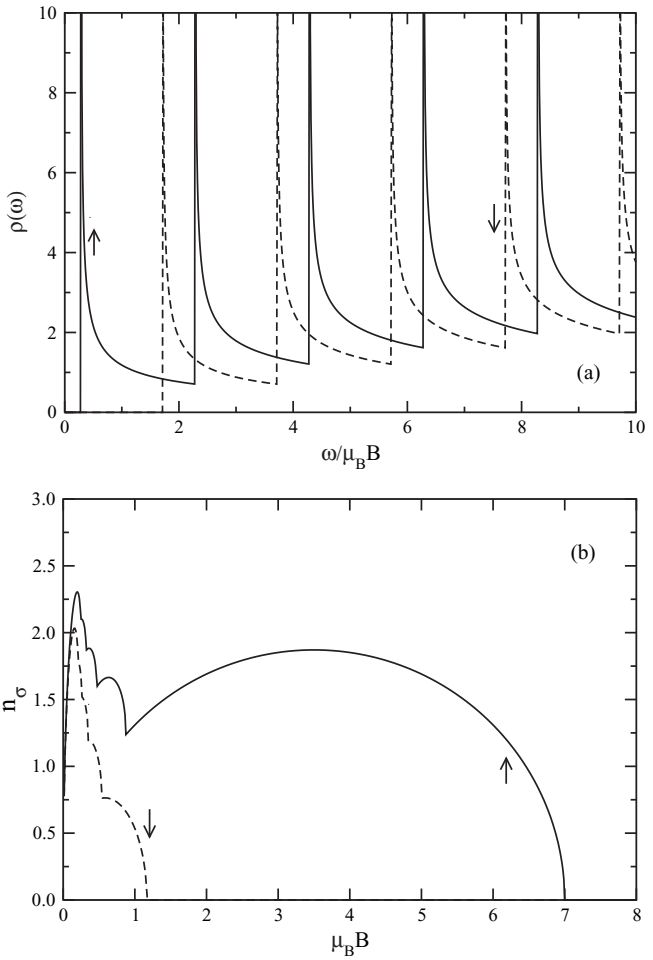

FIG. 2. (a) Density of states as a function of frequency over $\mu_B B$ for up-spin (solid curve) and down-spin (dashed curve) electrons displaying the one-dimensional van Hove singularities due to the Landau quantization. The DOS is given in units of $eB\sqrt{2m}/c(2\pi\hbar)^2$. (b) Occupation of the up-spin (solid curve) and down-spin (dashed curve) subband [in units of $2e\sqrt{2m}/\mu_B c(2\pi\hbar)^2$] as a function of $\mu_B B$ for chemical potential $\mu = 2$. As a consequence of the g factor, the lowest Landau level for the up-spins is the only occupied band for a large range of B.

In Eqs. (2) and (3), the contribution is zero if the argument of the square root is negative. Hence, the electron pocket is gradually emptied as a function of magnetic field with the down-spin subband being unoccupied first. As a consequence of the g factor being close to 2, there is a large field regime in which only the lowest Landau level in the up-spin subband is relevant [see Fig. 2(b)]. Hence, the Lifshitz transition as a function of field from partially filled to empty band takes place under complete spin polarization. Note that if we consider a hole band instead of an electron band, the band is filled rather than emptied with increasing field. Hence, the Lifshitz transition that is claimed to be a consequence of an emptying hole band in Refs. 6 and 8 should actually be an electron band. There is insufficient experimental evidence to distinguish the two cases.

One-dimensional van Hove singularities due a Lifshitz transition[9] have played a role in the statistical mechanics of numerous two-dimensional models.[16,17] For instance, an

array of flexible self-avoiding domain walls extending across a two-dimensional medium can be reduced to a one-dimensional fermion problem using transfer-matrix methods. With short-range interactions, the model can then be mapped onto a Heisenberg chain and has Luttinger liquid properties. For constant chemical potential, the equilibrium number of domain walls is a function of temperature and vanishes at $T_c(\mu)$ proportional to $[T - T_c(\mu)]^{1/2}$. The specific heat (proportional to the DOS) diverges with a square-root singularity at that point. Systems similar to this are of interest in connection with the wetting transition,[18] the commensurate-incommensurate transition,[19] the unbinding transition in membranes,[20] the statistics of "drunken walkers,"[21] etc.

III. INTERACTING ELECTRONS WITH LANDAU QUANTIZATION

The static density response function of the noninteracting electron gas $D^0(\mathbf{q},\omega = 0)$ in high fields at zero temperature exhibits logarithmic singularities for $q_z = q_{n,\sigma} + q_{n',\sigma}$, where q_z is the component of $\mathbf{q}$ parallel to the magnetic field and $q_{n,\sigma}$ is the Fermi momentum of the subband n,σ. These singularities indicate the tendency of the ground state to be unstable against the formation of charge-density waves with a wave vector parallel to the magnetic field. The perturbation expansion of the density response function $D(\mathbf{q},\omega = 0)$ in terms of a screened repulsive interaction potential yields logarithmic singularities of increasing order to all orders of perturbation. These logarithmic divergences have to be summed consistently to all orders of perturbation, which is best formulated in terms of parquet equations for the vertex function.

A. Parquet equations

The exact parquet equations for the electron gas in a high magnetic field have been considered in Refs. 12 and 13. The full vertex function $\Gamma(1,2,3,4)$ with the short-hand notation $1 = (\sigma_1,n_1,k_1^y,k_1^z,\omega_1)$, etc. (where σ is the spin component; n, k^y, and k^z are the usual quantum numbers in the Landau gauge; and ω is a fermion Matsubara frequency) can be decomposed into the sum of a totally irreducible part and three reducible blocks. Two of the reducible blocks are of the "zero-sound" type (reducible by cutting two antiparallel propagator lines) and the third one is the Cooper channel (reducible by cutting two parallel propagator lines). The parquet equations are integral equations for the reducible blocks with the irreducible diagrams as input. To leading logarithmic order it is sufficient to consider the bare vertex as the only irreducible input diagram, as long as the bare interaction is a screened Coulomb potential.

Within the leading logarithmic approximation, the k^z momenta and the frequency ω play the same role, namely, they become the logarithmic variable, η. This way the problem greatly simplifies and it can be reduced to one integro-differential equation for the vertex function, which still depends on two variables.[12] One variable is the logarithmic variable η with respect to which the equation is a differential one, and the other is $q_\perp$, the momentum in the plane perpendicular to the field, with respect to which it remains an integral equation. With respect to the logarithmic variable, this equation represents the renormalization-group equation, which arises when the electronic cutoff for the energy along the z direction is reduced. This equation could also be derived within Shankar's renormalization-group scheme[22] or the multiplicative renormalization.[23,24]

For an arbitrary bare repulsive interaction potential $V(q_z,q_\perp)$, the $q_\perp$ dependence introduces an additional length scale. With respect to q_z, we only need to consider two amplitudes, namely, the forward- and the backward-scattering amplitudes, corresponding to small momentum transfer and scattering across the Fermi surface. However, due to the $q_\perp$ dependence of the potential, the interaction depends on the component of the particle distance in the plane perpendicular to the field. This is the physical reason for the integro-differential equation, which can only be reduced to a pure differential one if the interaction is independent of the distance in the plane.[12]

B. Schulz-Keiter potential

Schulz and Keiter[13] proposed a potential that is independent of the particle distance in the plane perpendicular to the field, and hence the parquet equation would reduce to a differential equation.[12,14] The long-range interaction is then of the form

$$V(q_z,q_\perp) = w(q_z)L^2\delta_{q_\perp,0}, \tag{4}$$

where $\delta_{q_\perp,0}$ is a Kronecker delta. There are two relevant scattering processes, namely, small momentum transfer (forward scattering along the z direction) and scattering across the Fermi surface (backward scattering with $2q_{n,\sigma}$). Note that within the leading logarithmic approximation, only states with the same quantum numbers n and σ are relevant, so that we can suppress the indices of the Fermi momentum along the z direction. In particular, in the extreme quantum limit $n = 0$ and $\sigma = \uparrow$, and we denote the Fermi momentum with q_0. This condition is satisfied over a large range of fields [see Fig. 2(b)].

We denote $w(2q_0)$ by w_1 and $w(0)$ by w_2 and assume that only one energy or momentum variable, p, plays a relevant role in the vertex function (as is the case within the leading logarithmic approximation, see Ref. 12). This model can now be solved within the long-time approximation using bosonization techniques.[14] The vertex function has the structure

$$\Gamma_{k_1^z k_2^z k_3^z k_4^z}(p) = w_1\delta_{k_1^z k_3^z}\delta_{k_2^z k_4^z}\gamma_1(p) - w_2\delta_{k_1^z k_4^z}\delta_{k_2^z k_3^z}\gamma_2(p), \tag{5}$$

where γ_1 and γ_2 are vertex amplitudes that are independent of the k^z indices. The electron self-energy does not contribute to the leading logarithmic order, so that only perturbative corrections to the vertex need to be taken into account. To second order in the coupling they consist of the eight diagrams shown in Fig. 3, which are the same ones as for the 1D electron gas[23] and are straightforwardly evaluated.[14] Note that no spin index needs to be considered (the system is spin-polarized), but the Landau level degeneracy d has to be included. This degeneracy plays the same role as the spin index in the 1D gas. The resulting renormalization-group equations for the

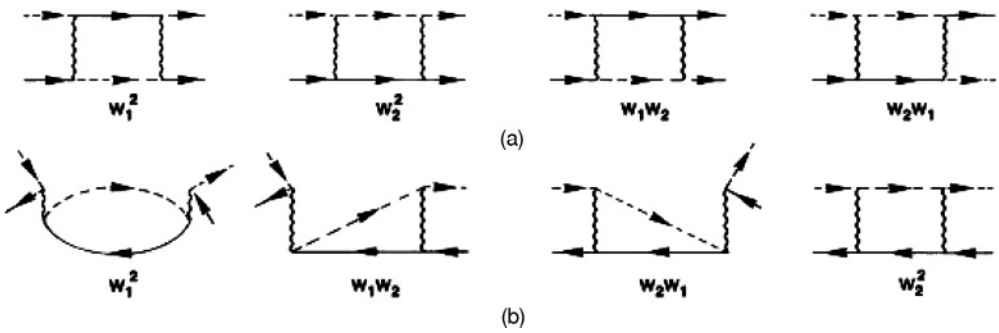

FIG. 3. Second-order vertex diagrams: (a) Cooper channel and (b) zero-sound channel. The full lines represent forward-moving particles, while the dashed lines correspond to backward movers.[14,23]

vertex amplitudes are now (obtained either via multiplicative renormalization[14] or by Shankar's method[22])

$$\frac{d\gamma_1}{d\eta} = -\kappa d w_1 \gamma_1^2, \qquad \frac{d\gamma_2}{d\eta} = -\kappa\left(w_1^2/w_2\right)\gamma_1^2, \tag{6}$$

where $\kappa = 1/(2\pi v_F) = m/(2\pi q_0)$. It is straightforward to see that one combination of invariant couplings is not renormalized, namely,

$$w_1\gamma_1 - d w_2\gamma_2 = w_1 - d w_2, \tag{7}$$

while the integration of the first of Eqs. (6) with the initial condition $\gamma_1(0) = 1$ yields

$$\gamma_1 = 1/[1 + \kappa d w_1 \eta]. \tag{8}$$

Hence, with increasing logarithmic variable η the vertex amplitude γ_1 renormalizes to zero. Although γ_1 renormalizes to zero, the system has the potential of being strongly coupled because the combination $w_1\gamma_1 - d w_2\gamma_2$ remains constant.

IV. DENSITY RESPONSE FUNCTION

The static uniform density response function is a measure of the change in the electron density as a response to an external charge perturbation, e.g., a change in the chemical potential. It is the quantity that determines how the lowest Landau level is populated when the chemical potential for the level is changed, for instance, by increasing the magnetic field.

To first order in perturbation with the Schulz-Keiter potential, the density response function is

$$D(\eta,q_\perp) = \frac{\kappa}{2\pi l^2}\exp\left[-\frac{1}{2}l^2q_\perp^2\right]\eta[1 - \kappa\eta(d w_1\delta_{q_\perp,0} - w_2)], \tag{9}$$

where $l = (L^2/2\pi d)^{1/2}$ is the magnetic length. Note that the density response function is discontinuous for $q_\perp = 0$, i.e., the value at $q_\perp = 0$ is different from the value at $q_\perp \to 0$. This discontinuity is a consequence of the long-ranged nature of the Schulz-Keiter interaction in the plane perpendicular to the magnetic field.

The function $D(\eta,q_\perp)$ does not satisfy the conditions for multiplicative renormalization.[23,24] We define the quantity

$$\overline{D}(\eta,q_\perp) = \frac{2\pi l^2}{\kappa}\exp\left[\frac{1}{2}l^2q_\perp^2\right]\frac{\partial}{\partial\eta}D(\eta,q_\perp) = 1 - 2\kappa\eta(d w_1\delta_{q_\perp,0} - w_2), \tag{10}$$

which has appropriate scaling behavior and satisfies the differential equation

$$\frac{\partial}{\partial\eta}\overline{D}(\eta,q_\perp) = 2\kappa[d w_1\delta_{q_\perp,0}\gamma_1(\eta) - w_2\gamma_2(\eta)], \tag{11}$$

with the initial condition $\overline{D}(\eta = 0,q_\perp) = 1$. The solution is

$$\overline{D}(\eta,q_\perp) = \exp[2\kappa(w_2 - w_1/d)\eta]/[1+d\kappa w_1\eta]^{2(\delta_{q_\perp,0}-1/d^2)}. \tag{12}$$

For $d = 2$ and $q_\perp = 0$, we recover Sólyom's result[24] for the 1D electron gas.

We need the homogeneous density response function, i.e., the $q_\perp = 0$ limit; the physically correct limit is $q_\perp \to 0$. Hence, the last factor in Eq. (12) is $[1 + d\kappa w_1\eta]^{2/d^2}$, which is only a very small correction to the exponential (note that the degeneracy d is very large) and can be neglected. Integrating $\overline{D}$ with respect to η, we obtain the density response function

$$D(\eta,q_\perp \to 0) \sim \frac{\exp[2\kappa(w_2 - w_1/d)\eta] - 1}{4\pi l^2(w_2 - w_1/d)}, \tag{13}$$

which has the exponential as the dominating feature. Hence, the system is strongly correlated as a consequence of the forward-scattering amplitude w_2. In Ref. 12, this divergence of $D(\eta,q_\perp)$ was interpreted as a possible instability to a charge-density wave or to a Wigner crystal phase. The new phase would have a characteristic length scale given by the inverse of the 1D Fermi momentum q_0.

We now return to the problem of the Lifshitz transition in the interacting system in a high magnetic field. The logarithmic variable η now has the form $\ln[(2q_0 + q_z)/(2q_0 - q_z)]$ and we must consider the limit $q_z \to 0$. Here q_z is the external momentum variable in the density correlation function and we need to consider the static and uniform limit of D, i.e., $\mathbf{q} = \mathbf{0}$ and $\omega = 0$. The logarithmic approximation is a consistent way of summing a specific class of diagrams, defined in Fig. 3. Without changing this resummation of diagrams, we can transform the argument of the logarithm without consequence

to the validity of the approximation. In other words, although as $q_z \to 0$ the logarithm no longer diverges, it still provides the same consistent diagram resummation.

Expression (13) now has the form

$$D(q_z \to 0, q_\perp \to 0) \sim \frac{\exp[(m/\pi q_0)(w_2 - w_1/d)] - 1}{4\pi l^2 (w_2 - w_1/d)}. \tag{14}$$

Close to the van Hove singularity, q_0 tends to zero so that the density correlation function diverges faster than a power law. As stated above, $D(\mathbf{q} = \mathbf{0}, z = 0)$ is the response of the number of carriers in the first Landau level to a change in the chemical potential or equivalently to a change in the magnetic field. The integral of the correlation function with respect to q_0 yields the change in the number of particles in the band. However, the singularity we obtained is not integrable, so that the change in the number of particles when the band starts to get filled is discontinuous. The system is strongly interacting and the continuous filling of the noninteracting van Hove singularity [$n \sim (\omega - \mu)^{1/2}$] is changed to a discontinuous one by the Coulomb interaction at $T = 0$. With the carrier density calculated in linear response, it is not possible to determine the magnitude of the jump. Although the Schulz-Keiter interaction is long-ranged in the plane perpendicular to the field (so that the integro-differential parquet equations can be reduced to pure differential ones) and hence somewhat peculiar, we do not expect the general property of strong coupling to change for a more realistic interaction potential.

At finite temperature, the smearing of the Fermi surface prevents the density correlation function from diverging. In the vertex amplitudes, the logarithmic variable η is to be replaced by

$$\eta = \ln\left(\frac{4q_0}{|p|}\right) \to \ln\left(\frac{4q_0}{4\pi T}\right) - \mathrm{Re}\psi\left(\frac{1}{2} + i\frac{p}{4\pi T}\right), \tag{15}$$

where Re denotes the real part and ψ is the digamma function. A similar replacement is in order in the density function, namely,

$$\eta = \ln\left(\frac{2q_0 + q_z}{2q_0 - q_z}\right) \to \mathrm{Re}\psi\left(\frac{1}{2} + i\frac{2q_0 + q_z}{4\pi T}\right) - \mathrm{Re}\psi\left(\frac{1}{2} + i\frac{2q_0 - q_z}{4\pi T}\right), \tag{16}$$

which expanded for small q_z yields

$$-\frac{2q_z}{4\pi T}\mathrm{Im}\psi'\left(\frac{1}{2} + i\frac{2q_0}{4\pi T}\right), \tag{17}$$

where Im denotes the imaginary part and ψ' is the trigamma function. In the limit $T \to 0$, Eq. (17) reduces to q_z/q_0. Hence, expression (17) divided by q_z replaces $1/q_0$ in Eq. (14). This way at low but finite T the correlation function no longer diverges as $q_0 \to 0$. Two regimes have to be distinguished: (i) $T > q_0$, where Eq. (17) is proportional to $q_0 q_z/(2\pi T)^2$, and (ii) $T < q_0$, where Eq. (17) reduces to q_z/q_0. The two regimes are separated by a crossover region.

Due to the absence of divergence of the density correlation function at finite T, the filling of the first Landau level is continuous as a function of field. Instead of a square root dependence of the occupation as a function of B, there is a strong increase at low T when q_0 is passing the crossover region and a sharp peak when regime (ii) is reached. The height of the peak increases as $T \to 0$ until the transition is discontinuous at $T = 0$. This behavior is consistent with the experimental findings for $CeIn_3$,[10] where a continuous transition has been found in a TDO probe measurement that becomes a jump when extrapolated to $T \to 0$. Hence, the combination of Landau quantization and Coulomb interaction gives rise to a strong-coupling situation that leads to the modification of the standard Lifshitz transition.

V. CONCLUSIONS

Using the leading logarithmic solution of the Schulz-Keiter model in the presence of strong Landau quantization, we have studied the Lifshitz transition for a heavy electron band as a function of magnetic field at constant chemical potential (coupling to an electron reservoir). For the free-electron gas in a strong magnetic field, the Landau quantization modifies the dimensionality of the 3D Lifshitz transition to one with 1D characteristics. Repulsive electron-electron interactions further change the nature of the transition to one that is discontinuous at $T = 0$. This discontinuity is gradually smeared at finite T, in agreement with experimental observations. Although the Schulz-Keiter interaction has a peculiar long-range potential form within the plane perpendicular to the magnetic field, we do not expect this result to be affected qualitatively. The magnetic-field dependence of the Lifshitz transition also suggests that the transition of $CeIn_3$ corresponds to an electron rather than a hole pocket.

Note that disorder can also affect the states close to a van Hove singularity, which could become localized at the band edge. A mobility edge separates the localized from the extended states, and only if the chemical potential lies above the mobility edge can the states contribute to conduction. There are four arguments discarding disorder as the possible cause for the effect discussed here. (i) The samples are of very high purity, so that a mobility edge should not arise. (ii) There are other conductive states (represented by the reservoir pinning the chemical potential), which would screen the effects of disorder. (iii) Disorder would not give rise to a discontinuity of the skin depth in the ground state as a function of field. (iv) The temperature dependence of the skin depth would be less remarkable close to the disorder insulator-metal transition.

ACKNOWLEDGMENTS

The support of the US Department of Energy under Grants No. DE-FG02-98ER45707 and No. NNSA DE-FG52-10NA29659 is acknowledged.

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