Low-temperature theory of inversion and quantum oscillations in Kondo insulators

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The half-filled Kondo lattice model is studied at low temperatures on a simple cubic lattice using the self-consistent theory developed by Ram and Kumar [Phys. Rev. B **96**, 075115 (2017)]. It is found to have three distinct insulating phases in the temperature-hopping plane, namely, the strong-coupling Kondo singlet (KS) phase, the inverted Kondo singlet (iKS) phase distinguished from the KS by inversion, and the antiferromagnetic (AFM) phase. The quasiparticle density of states across the inversion transition is noted to exhibit a dimensional reduction, which can differentiate between the KS and iKS insulators in experiments. Magnetic quantum oscillations obtained in the iKS and AFM phases are found to show a Lifshitz-Kosevich-like behavior with temperature as well as quantum fluctuations induced by the Kondo interaction.

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I. INTRODUCTION

Kondo insulators are heavy fermion systems commonly realized in rare-earth compounds [1,2]. They behave as insulators at low temperatures due to the interaction of itinerant electrons with local moments. Recent observations of quantum oscillations in two well-known Kondo insulators, SmB_6 [3–5] and YbB_{12} [6–8], have led to a surge of interest in the subject. Quantum oscillations of quantities such as magnetization in response to a magnetic field have for long been considered a characteristic of metals [9]. These observations challenge that. Different scenarios and theories have been put forward in recent years to understand this intriguing situation of Kondo insulators exhibiting quantum oscillations [10–20].

Of particular interest to us in this paper is a theory of Kondo insulators put forward in Ref. [15]. Notably, it finds that the dispersion of the gapped charge quasiparticles undergoes inversion upon decreasing the Kondo coupling, and the quantum oscillations in the insulating bulk appear only after the inversion has occurred. This inversion is a genuine many-body effect resulting from the competition between the Kondo interaction J and the conduction electron hopping t. For small t/J, i.e., strong Kondo couplings, the charge gap comes from the center of the Brillouin zone. But upon increasing t/J beyond the so-called inversion point, the zone center becomes a local maximum and the charge gap shifts to a surface around the zone center. Across this inversion transition, the ground state remains a Kondo singlet. A further increase in t/J leads to antiferromagnetic ordering.

This theory elucidates the microscopic basis for the existence of quantum oscillations in the insulating bulk by discovering many-body inversion as a key property of the correlated insulators. It was nicely worked out for two prototypical models of Kondo insulators, viz., the half-filled Kondo lattice model [15] and the symmetric periodic Anderson model [17] in the ground state, i.e., at absolute zero temperature. What happens to the inversion, and the consequent possibility of quantum oscillations, at finite temperatures remains to be understood. It is our goal here to address this question.

In this paper, we extend the theory enunciated in Ref. [15] to finite temperatures, and study the behavior of inversion and quantum oscillations in the half-filled Kondo lattice model (KLM) on a simple cubic lattice. We present the theory in Sec. II, and obtain the phase diagram in the temperature-hopping plane. Notably, we get an inversion transition also at finite temperatures, with an "inverted" Kondo singlet phase in an extended region of the phase diagram. We also identify characteristic changes in the quasiparticle density of states and specific heat across the inversion transition that can experimentally differentiate between the Kondo insulators distinguished by inversion. In Sec. III, we study magnetic quantum oscillations at finite temperatures. We get these oscillations in the inverted Kondo singlet as well as antiferromagnetic phases, and find them to follow a Lifshitz-Kosevich-like behavior with respect to temperature as well as J^2/t. We conclude this paper with a summary in Sec. IV.

II. HALF-FILLED KONDO LATTICE MODEL

The Kondo lattice model (KLM)

$$\mathcal{H} = -t\sum_{\vec{r},\vec{\delta}}\sum_{s=\uparrow,\downarrow}\hat{c}^{\dagger}_{\vec{r},s}\hat{c}_{\vec{r}+\vec{\delta},s} + \frac{J}{2}\sum_{\vec{r}}\vec{S}_{\vec{r}}\cdot\vec{\tau}_{\vec{r}} \tag{1}$$

of local moments coupled antiferromagnetically ($J > 0$) to the electrons of a half-filled conduction band describes Kondo insulators. On bipartite lattices with nearest-neighbor hopping t, exact half filling is ensured by zero chemical potential. Here, we consider a simple cubic lattice formed by L sites with position vectors $\{\vec{r}\}$; $\vec{\delta}$ denotes the nearest neighbors of every point $\vec{r}$. The local moments are described by the Pauli operators $\vec{\tau}_{\vec{r}}$'s while $\hat{c}_{\vec{r},s}$ ($\hat{c}^{\dagger}_{\vec{r},s}$) and $\vec{S}_{\vec{r}}$ denote respectively the annihilation (creation) and spin operators of the conduction electrons.

In Ref. [15], a self-consistent theory of Kondo insulators was formulated in the Kumar representation of electrons [21]:

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$\hat{c}^\dagger_{\vec{r}\uparrow} = \hat{\phi}_{a,\vec{r}}\,\sigma^+_{\vec{r}}$, $\hat{c}^\dagger_{\vec{r}\downarrow} = \frac{1}{2}(i\psi_{a,\vec{r}} - \phi_{a,\vec{r}}\,\sigma^z_{\vec{r}})$ on the A sublattice and $\hat{c}^\dagger_{\vec{r},\uparrow} = i\hat{\psi}_{b,\vec{r}}\,\sigma^+_{\vec{r}}$, $\hat{c}^\dagger_{\vec{r},\downarrow} = \frac{1}{2}(\phi_{b,\vec{r}} - i\psi_{b,\vec{r}}\,\sigma^z_{\vec{r}})$ on the B sublattice; here, $\phi_{a(b),\vec{r}}$, $\psi_{a(b)\vec{r}}$ are the Majorana fermion operators and $\sigma^z_{\vec{r}}, \sigma^\pm_{\vec{r}}$ are the Pauli operators. Following Ref. [15], the half-filled KLM is written as $\mathcal{H} \approx \mathcal{H}_c + \mathcal{H}_s + e_0 L$, where

$$\mathcal{H}_c = \frac{J\rho_0}{4}\left(\sum_{\vec{r}\in A}\hat{a}^\dagger_{\vec{r}}\,\hat{a}_{\vec{r}} + \sum_{\vec{r}\in B}\hat{b}^\dagger_{\vec{r}}\,\hat{b}_{\vec{r}}\right) - \frac{it}{2}\sum_{\vec{r}\in A}\sum_{\vec{\delta}}(\psi_{a,\vec{r}}\,\phi_{b,\vec{r}+\vec{\delta}} + \rho_1\psi_{b,\vec{r}+\vec{\delta}}\,\phi_{a,\vec{r}}) \tag{2a}$$

$$= \frac{J\rho_0 L}{8} + \sum_{\vec{k}}\sum_{\nu=\pm}E_{\vec{k},\nu}\left(\eta^\dagger_{\vec{k},\nu}\eta_{\vec{k},\nu} - \frac{1}{2}\right) \tag{2b}$$

describes the effective "charge" dynamics in terms of the spinless fermions $\hat{a}_{\vec{r}}$ and $\hat{b}_{\vec{r}}$ such that $\phi_{a,\vec{r}} = \hat{a}_{\vec{r}} + \hat{a}^\dagger_{\vec{r}}$ and $\psi_{a,\vec{r}} = i(\hat{a}_{\vec{r}} - \hat{a}^\dagger_{\vec{r}})$ on the A sublattice, and $\phi_{b,\vec{r}} = \hat{b}_{\vec{r}} + \hat{b}^\dagger_{\vec{r}}$ and $\psi_{b,\vec{r}} = i(\hat{b}_{\vec{r}} - \hat{b}^\dagger_{\vec{r}})$ on the B sublattice; the parameters ρ_0 and ρ_1 defined below are to be determined self-consistently. After doing Fourier and Bogoliubov transformations of the spinless fermions, we obtain Eq. (2b) from Eq. (2a), where $\eta_{\vec{k},\nu}$ are the quasiparticle operators corresponding to the $\vec{k}$ points in the half-Brillouin zone, and $E_{\vec{k},\pm} = E_{\vec{k}} \pm \frac{1}{2}t(1+\rho_1)|\gamma_{\vec{k}}|$ are the quasiparticle dispersions; here, $\gamma_{\vec{k}} = \sum_{\vec{\delta}} e^{i\vec{k}\cdot\vec{\delta}}$ and $E_{\vec{k}} = \sqrt{(J\rho_0/4)^2 + [t(1-\rho_1)|\gamma_{\vec{k}}|/2]^2}$. The "spin" physics of the half-filled KLM is described effectively by the following model,

$$\mathcal{H}_s = \frac{J\bar{n}}{4}\sum_{\vec{r}}\vec{\sigma}_{\vec{r}}\cdot\vec{\tau}_{\vec{r}} + \frac{t\zeta}{4}\sum_{\vec{r},\vec{\delta}}\vec{\sigma}_{\vec{r}}\cdot\vec{\sigma}_{\vec{r}+\vec{\delta}}. \tag{3a}$$

The four self-consistent parameters of this theory are defined as $\rho_0 = \frac{1}{L}\sum_{\vec{r}}\langle\vec{\sigma}_{\vec{r}}\cdot\vec{\tau}_{\vec{r}}\rangle$, $\rho_1 = \frac{1}{zL}\sum_{\vec{r},\vec{\delta}}\langle\vec{\sigma}_{\vec{r}}\cdot\vec{\sigma}_{\vec{r}+\vec{\delta}}\rangle$, $\zeta = \frac{2i}{zL}\sum_{\vec{r}\in A,\vec{\delta}}\langle\phi_{a,\vec{r}}\psi_{b,\vec{r}+\vec{\delta}}\rangle$, $\bar{n} = \frac{1}{L}\langle\sum_{\vec{r}\in A}\hat{a}^\dagger_{\vec{r}}\hat{a}_{\vec{r}} + \sum_{\vec{r}\in B}\hat{b}^\dagger_{\vec{r}}\hat{b}_{\vec{r}}\rangle$. The constant term is $e_0 = -(J\bar{n}\rho_0 + zt\zeta\rho_1)/4$. We urge the readers to look at Ref. [15] for more details.

The $\mathcal{H}_s$ is a hard problem. At the simplest analytical level, we treat $\mathcal{H}_s$ using bond-operator mean-field theory [22] in terms of the singlet and triplet eigenstates of the local interaction, $J\vec{\sigma}_{\vec{r}}\cdot\vec{\tau}_{\vec{r}}$. It amounts to writing the Pauli operators approximately as $\sigma_{\vec{r},\alpha} \approx \bar{s}(\hat{t}^\dagger_{\vec{r},\alpha} + \hat{t}_{\vec{r},\alpha}) \approx -\tau_{\vec{r},\alpha}$ for $\alpha = x, y, z$; here, $\bar{s}^2$ is the weight of a Kondo singlet per site, and the boson operators $\hat{t}_{\vec{r},\alpha}$ describe the triplet excitations. By doing Fourier and Bogoliubov transformations of these bosons, we obtain the following diagonalized form of $\mathcal{H}_s$ with triplon dispersion, $\epsilon_{\vec{k}} = \sqrt{\lambda(\lambda + t\zeta\bar{s}^2\gamma_{\vec{k}})}$, for the $\vec{k}$ points in the full Brillouin zone; here, λ is the Lagrange multiplier that enforces on average the physical constraint, $\bar{s}^2 + \sum_\alpha \hat{t}^\dagger_{\vec{r},\alpha}\hat{t}_{\vec{r},\alpha} = 1$:

$$\mathcal{H}_s \approx L\left[\lambda\bar{s}^2 - \frac{5\lambda}{2} + \frac{J\bar{n}\rho_0}{4}\right] + \sum_{\vec{k},\alpha}\epsilon_{\vec{k}}\left(\tilde{t}^\dagger_{\vec{k},\alpha}\tilde{t}_{\vec{k},\alpha} + \frac{1}{2}\right). \tag{3b}$$

A. Self-consistent equations at finite temperatures

The parameters ρ_0, ρ_1, ζ, $\bar{n}$ of this theory are to be determined self-consistently. In Ref. [15], these calculations were done at temperature $T = 0$ only. Here, we do so at finite T to understand how with temperature the inversion and quantum oscillations behave in this theory. Equations for ζ and $\bar{n}$, obtained by thermal averaging the related operators (defined above) with respect to Eq. (2b), are written below; here, $\beta = 1/T$:

$$\bar{n} = \frac{1}{2} - \frac{J\rho_0}{8L}\sum_{\vec{k},\nu}\frac{\tanh(\beta E_{\vec{k},\nu}/2)}{E_{\vec{k}}}, \tag{4a}$$

$$\zeta = \frac{1}{zL}\sum_{\vec{k},\nu}|\gamma_{\vec{k}}|\left[\frac{t(1-\rho_1)|\gamma_{\vec{k}}|}{2E_{\vec{k}}} - \nu\right]\tanh(\beta E_{\vec{k},\nu}/2). \tag{4b}$$

By minimizing with respect to $\bar{s}^2$ and λ the free energy, $\mathcal{F}_s = -\frac{1}{\beta}\log\mathrm{tr}\,e^{-\beta\mathcal{H}_s}$, obtained from Eq. (3b), we get the following equations in the gapped singlet phase:

$$\bar{s}^2 = \frac{5}{2} - \frac{3}{4L}\sum_{k}\frac{2\lambda + t\zeta\bar{s}^2\gamma_{\vec{k}}}{\epsilon_{\vec{k}}}\coth(\beta\epsilon_{\vec{k}}/2), \tag{5a}$$

$$\lambda = J\bar{n} - \frac{3t\zeta\lambda}{4L}\sum_{\vec{k}}\frac{\gamma_{\vec{k}}}{\epsilon_{\vec{k}}}\coth(\beta\epsilon_{\vec{k}}/2). \tag{5b}$$

In the gapless antiferromagnetic phase, $\epsilon_{\vec{Q}} = 0$ at $\vec{Q} = (\frac{\pi}{a}, \frac{\pi}{a}, \frac{\pi}{a})$; here, a denotes the lattice constant. It gives $\lambda = zt\zeta\bar{s}^2$, and modifies Eq. (5a) to

$$\bar{s}^2 = \frac{5}{2} - n_c - \frac{3}{4L}\sum_{\vec{k}\neq\vec{Q}}\frac{2\lambda + t\zeta\bar{s}^2\gamma_{\vec{k}}}{\epsilon_{\vec{k}}}\coth(\beta\epsilon_{\vec{k}}/2), \tag{6a}$$

with condensate density n_c accounting for order [23]:

$$n_c = \frac{1}{t\zeta z}\left[\lambda - J\bar{n} + \frac{3t\zeta\lambda}{4L}\sum_{k\neq Q}\frac{\gamma_k}{\epsilon_k}\coth(\beta\epsilon_k/2)\right]. \tag{6b}$$

From these, we get $\rho_0 = 1 - 4\bar{s}^2$ and $\rho_1 = \frac{4\bar{s}^2(J\bar{n}-\lambda)}{zt\zeta}$.

B. Phase diagram

By solving Eqs. (4a)–(5b) self-consistently for $\bar{n}$, ζ, ρ_0, and ρ_1, we obtain the charge and spin dispersions and the respective energy gaps as a function of t and T in units of J. At $T = 0$, we get the results known from Ref. [15]. Namely, upon increasing t, the inversion of charge dispersion starts at $t_i = 0.33$, and the spin gap closes continuously at $t_c = 0.62$, causing a transition from the singlet phase to antiferromagnetic (AFM) phase [24]. For $t < t_i$ the charge gap comes from the zone center, $\vec{k} = 0$, while for $t > t_i$, it comes from the surface, $\gamma_{\vec{k}} = \frac{J|\rho_0|(1-|\rho_1|)}{4t(1+|\rho_1|)\sqrt{|\rho_1|}}$, that quickly tends to $\gamma_{\vec{k}} = 0$ as t increases. By tracing the evolution of the inversion point t_i and the antiferromagnetic critical point t_c with temperature, we get a phase diagram in the t-T plane, as presented in Fig. 1. Inside the antiferromagnetic phase, we use Eqs. (6a) and (6b) together with Eqs. (4a) and (4b) to find the solution.

At low temperatures, we find the half-filled KLM to have three distinct insulating phases separated by the inversion line $t_i(T)$ and the AFM phase boundary $t_c(T)$. Across the inversion transition (dotted line in Fig. 1), the spins continue to form a singlet, but the charge dispersion exhibits a change in the form of inversion. Thus, we call the strong-coupling singlet phase for $t < t_i$ simply as the Kondo singlet (KS) phase, while that for $t_i < t < t_c$ as the inverted Kondo singlet (iKS) phase;

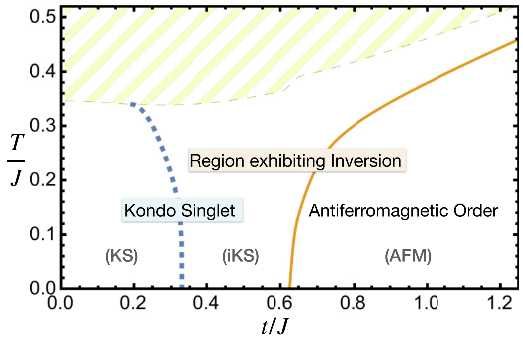

FIG. 1. Phase diagram of the half-filled Kondo lattice model in the hopping (t)-temperature (T) plane in units of Kondo interaction (J). It has three low-temperature insulating phases: a strong-coupling Kondo singlet (KS), inverted Kondo singlet (iKS), and the antiferromagnetic (AFM) phase. The dotted line marks the inversion transition. The continuous line marks the antiferromagnetic transition. The hatched region marks the limitation of the present treatment of $\mathcal{H}_s$ for higher temperatures.

the AFM phase enveloped by the iKS phase lies entirely in the region exhibiting inversion. Notably, the iKS phase is found to grow in extent upon increasing T. It implies that the real Kondo insulators with not-so-strong Kondo couplings would invariably realize the iKS phase. It has important consequences for the quantum oscillations at finite temperatures; as figured out in Ref. [15], inversion is a necessary condition for the quantum oscillation to occur in the Kondo insulating bulk.

Across the inversion transition, the quasiparticle density of states (DOS) near the charge gap Δ_c exhibits a notable change in the behavior from $(E-\Delta_c)^{1/2}$ in the KS phase to $(E-\Delta_c)^{-1/2}$ in the iKS phase; see Fig. 2. It is so caused by the dimensional reduction of dispersion near Δ_c. The low-energy dispersion in the KS phase, $E_{\vec{k},-}-\Delta_c \sim |\vec{k}|^2$, is fully three dimensional around the zone center, whereas in the iKS phase, $E_{\vec{k},-}-\Delta_c \sim k_\perp^2$ is effectively one dimensional because the energy close to Δ_c increases only along the normal to the gap surface; $k_\perp$ is the component of $\vec{k} \perp$ to the gap surface.

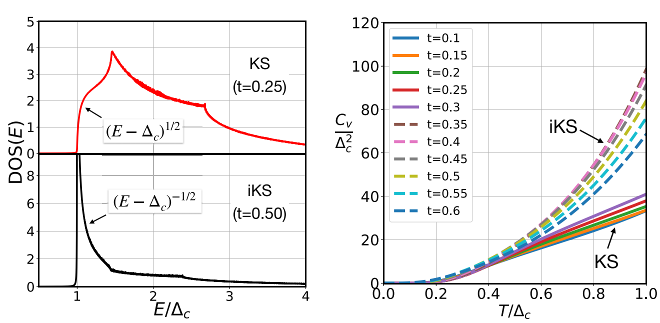

FIG. 2. Left: Quasiparticle density of states (DOS) at $T=0$. Right: Specific heat C_v. Note the change in behavior of DOS from $(E-\Delta_c)^{1/2}$ in the KS phase to $(E-\Delta_c)^{-1/2}$ in the iKS phase, near the charge gap Δ_c. It amounts to enhancing C_v in the iKS phase. Also note the bunching of specific-heat data into two groups corresponding to KS and iKS, when plotted as C_v/Δ_c^2 vs T/Δ_c; here, Δ_c is T dependent.

This change in DOS would show up in physical quantities such as the specific heat C_v. In the two types of Kondo insulators distinguished by inversion, the specific heat at low enough temperatures is expected to behave as

$$C_v \sim \Delta_c^2\, e^{-\Delta_c/T} \times \begin{cases} T^{-\frac{1}{2}} & \text{(for KS insulators),} \\ T^{-\frac{3}{2}} & \text{(for iKS insulators).} \end{cases} \tag{7}$$

Since this difference arises due to inversion, it can be used experimentally to differentiate between the two types of Kondo insulators. In both cases, C_v scales as Δ_c^2. Hence, C_v/Δ_c^2 vs T/Δ_c for different Kondo insulators would form two bunches corresponding to KS and iKS types, as the calculated specific heat in Fig. 2 shows. (Notably, the specific heat for iKS insulators has the BCS form [25]; the two behave similarly for the same reason, although they describe different phenomena.)

Upon increasing T further, we hit the boundary of the hatched region in Fig. 1, whereafter finding the self-consistent solutions of Eqs. (5a) and (5b) becomes difficult; for small t/J, it happens where the crossover from the KS to thermal paramagnetic insulator is expected ($T/J \sim 0.375$), and for larger t/J, it happens where the iKS insulator to metal transition is expected. This difficulty arises due to the approximation $\bar{s}$ for local singlets, which is fine at low but not at high temperatures. It calls for other ways of treating $\mathcal{H}_s$ to access high-temperature phases within this theory. The present approach describes the low-temperature insulating phases of the half-filled KLM in good detail.

III. MAGNETIC QUANTUM OSCILLATIONS

We now study the dynamics of charge quasiparticles in magnetic field, and investigate the behavior of quantum oscillations at low temperatures. As in Ref. [15], we do it by the following minimal finite-field extension of the zero field $\mathcal{H}_c$ of Eq. (2a):

$$\mathcal{H}_{c,\alpha} = \frac{J\rho_0}{4}\left(\sum_{\vec{r}\in A}\hat{a}_{\vec{r}}^\dagger\,\hat{a}_{\vec{r}} + \sum_{\vec{r}\in B}\hat{b}_{\vec{r}}^\dagger\,\hat{b}_{\vec{r}}\right) - \frac{it}{2}\sum_{\vec{r}\in A}\sum_{\vec{\delta}} \times \cos(2\pi\alpha\, r_y\,\hat{x}\cdot\hat{\delta})[\psi_{a,\vec{r}}\,\phi_{b,\vec{r}+\vec{\delta}} + \rho_1\psi_{b,\vec{r}+\vec{\delta}}\,\phi_{a,\vec{r}}]. \tag{8}$$

Here, $\alpha = Ba^2/(e/h)$ is the magnetic flux in units of e/h for magnetic field B along the z direction (described by the vector potential $\vec{A} = -yB\hat{x}$ along the x direction), and r_y is the y component of $\vec{r}$. In numerical calculations, α is taken as p/q, with $p = 1, 2 \ldots q$ for a prime number q; we take $q = 503$. We diagonalize $\mathcal{H}_{c,\alpha}$ numerically for different values of α for several different T's and t's by putting in Eq. (8) the corresponding zero-field values of ρ_0 and ρ_1. We then calculate its free energy $\mathcal{F}_c(\alpha, T, t)$ and obtain from it the magnetization $\mathcal{M} = -(\partial\mathcal{F}_c/\partial\alpha)/L$.

In Fig. 3, we present the magnetization data thus calculated. As in the ground state [15], we get oscillations in $\mathcal{M}/\alpha$ with $1/\alpha$ also at finite temperatures; with backgrounds subtracted, the oscillations die off to zero. These oscillations occur only in the inverted region; they grow in strength by increasing hopping, but weaken by increasing temperature. For t around 0.7, we begin to see clear magnetic quantum oscillations. The iKS phase at such hopping values occurs invariably at higher temperatures, so the oscillations seen in

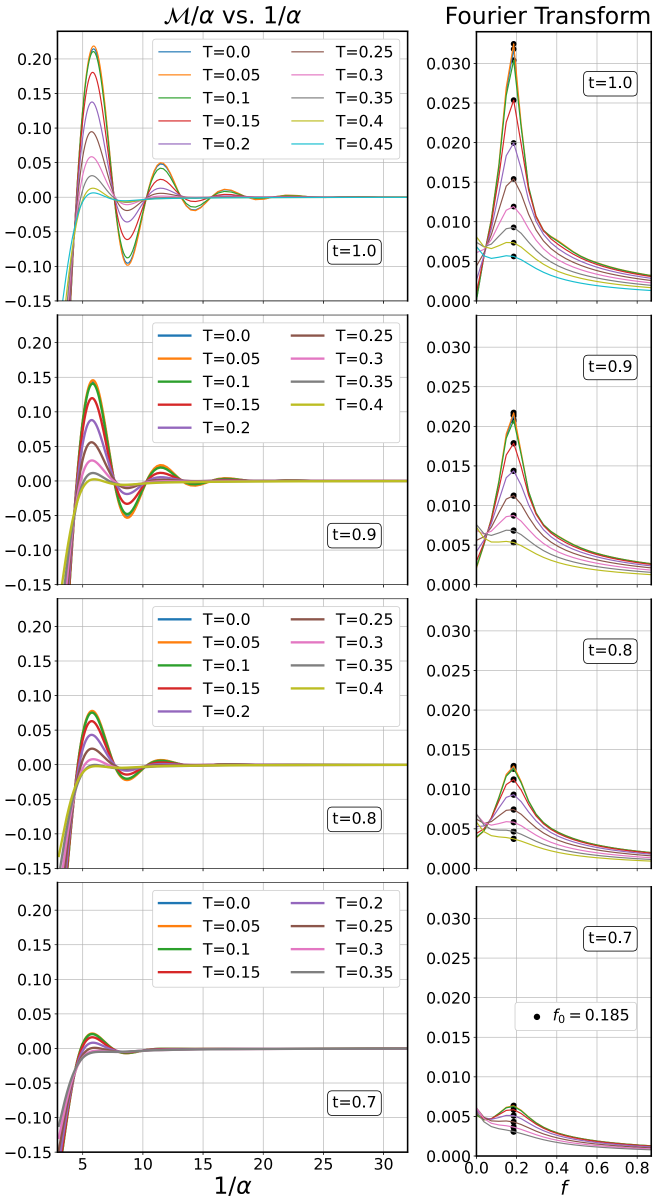

FIG. 3. Magnetic quantum oscillations obtained from our calculations. They oscillate with frequency $f_0 = 0.185$, and weaken by increasing temperature or decreasing hopping. (The same color code applies to the data in the plots on the left and the right for the same t.)

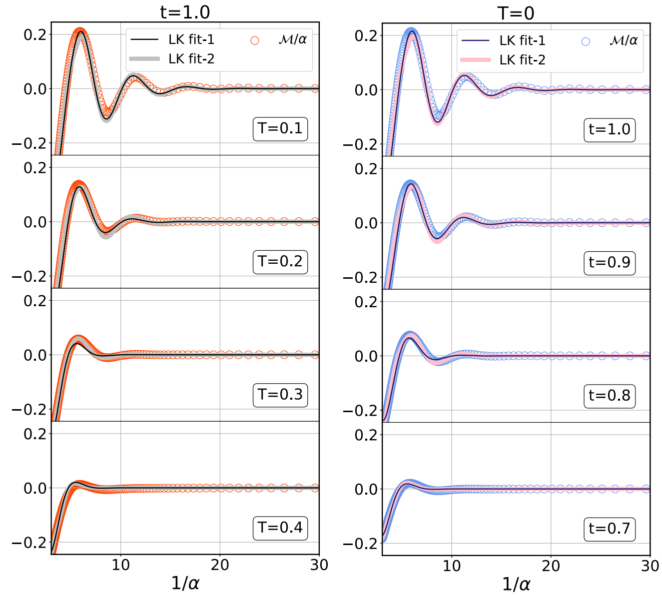

FIG. 4. Magnetic oscillations fitted with the Lifshitz-Kosevich (LK) form for frequency $f_0 = 0.185$. A two-parameter fit (LK fit-1) with only the first two terms of the formula already looks good. LK fit-2 is a five-parameter fit involving the first four terms.

the iKS phase are weaker compared to those seen in the AFM phase, but they are unmistakably there on both sides of the iKS-AFM phase boundary. Fourier transforming this magnetization data gives the oscillation frequency $f_0 = 0.185$; it has been identified to correspond to a contour on the $\gamma_{\vec{k}} = 0$ surface in the bulk Brillouin zone [15]. We fit the calculated magnetization with the Lifshitz-Kosevich (LK) formula $\mathcal{M} = \frac{T}{\sqrt{\alpha}} \sum_n c_n (-1)^{n+1} \frac{\sin[(2\pi n f_0/\alpha)+(\pi/4)]}{\sqrt{n}\sinh(nbT/\alpha)}$ [9,26]; ideally, the c_n's are all equal, say c. We find that an LK fit with only two parameters b and c, and the first two terms of the series, already describes these oscillations remarkably well with respect to T. See Fig. 4. This is consistent with experiments; in YbB_{12}, the LK behavior is observed down to 60 mK [6,7], and in SmB_6 down to about 1 K [4,5]. Notably, if we replace T in this formula by $1/t$, it describes very well the oscillations at $T = 0$. In dimensionful terms, it means that J^2/t acts effectively as temperature. Hence, we find that the Kondo insulating bulk not only exhibits quantum oscillations, but it does so in a Lifshitz-Kosevich-like manner with temperature as well as the Kondo interaction-induced quantum fluctuations through a Ruderman-Kittel-Kasuya-Yosida (RKKY)-like parameter J^2/t.

IV. SUMMARY

We have described a low-temperature theory of inversion and quantum oscillations in the half-filled Kondo lattice model on a simple cubic lattice with implications for real Kondo insulators. The key takeaways from this paper are as follows. The Kondo insulators come in two types, the KS (Kondo singlet) and iKS (inverted Kondo singlet), distinguished by inversion. They can be differentiated by spectral or specific-heat measurements, as they have a different density of states near the charge gap. The iKS insulators can also realize AFM (antiferromagnetic) order by increasing hopping (say, pressure) or decreasing temperature. Magnetic quantum oscillations occur in the bulk of the inverted Kondo insulators (iKS as well as AFM), and they follow Lifshitz-Kosevich behavior with respect to temperature as well as J^2/t.

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[1] C. M. Varma, Mixed-valence compounds, Rev. Mod. Phys. **48**, 219 (1976).
[2] P. Misra, *Heavy-Fermion Systems* (Elsevier, Amsterdam, 2008).
[3] G. Li, Z. Xiang, F. Yu, T. Asaba, B. Lawson, P. Cai, C. Tinsman, A. Berkley, S. Wolgast, Y. S. Eo *et al.*, Two-dimensional Fermi surfaces in Kondo insulator SmB_6, Science **346**, 1208 (2014).
[4] B. Tan, Y.-T. Hsu, B. Zeng, M. C. Hatnean, N. Harrison, Z. Zhu, M. Hartstein, M. Kiourlappou, A. Srivastava, M. Johannes *et al.*, Unconventional Fermi surface in an insulating state, Science **349**, 287 (2015).
[5] M. Hartstein, W. Toews, Y.-T. Hsu, B. Zeng, X. Chen, M. C. Hatnean, Q. Zhang, S. Nakamura, A. Padgett, G. Rodway-Gant *et al.*, Fermi surface in the absence of a Fermi liquid in the Kondo insulator SmB_6, Nat. Phys. **14**, 166 (2018).
[6] H. Liu, M. Hartstein, G. J. Wallace, A. J. Davies, M. C. Hatnean, M. D. Johannes, N. Shitsevalova, G. Balakrishnan, and S. E. Sebastian, Fermi surfaces in Kondo insulators, J. Phys.: Condens. Matter **30**, 16LT01 (2018).
[7] Z. Xiang, Y. Kasahara, T. Asaba, B. Lawson, C. Tinsman, L. Chen, K. Sugimoto, S. Kawaguchi, Y. Sato, G. Li, S. Yao, Y. L. Chen, F. Iga, J. Singleton, Y. Matsuda, and L. Li, Quantum oscillations of electrical resistivity in an insulator, Science **362**, 65 (2018).
[8] N. P. Ong, Quantum oscillations in an insulator, Science **362**, 32 (2018).
[9] D. Shoenberg, *Magnetic Oscillations in Metals*, Cambridge Monographs on Physics (Cambridge University Press, Cambridge, UK, 1984).
[10] J. Knolle and N. R. Cooper, Quantum Oscillations without a Fermi Surface and the Anomalous de Haas–van Alphen Effect, Phys. Rev. Lett. **115**, 146401 (2015).
[11] G. Baskaran, Majorana Fermi sea in insulating SmB_6: A proposal and a theory of quantum oscillations in Kondo insulators, arXiv:1507.03477.
[12] L. Zhang, X.-Y. Song, and F. Wang, Quantum Oscillation in Narrow-Gap Topological Insulators, Phys. Rev. Lett. **116**, 046404 (2016).
[13] O. Erten, P. Ghaemi, and P. Coleman, Kondo Breakdown and Quantum Oscillations in SmB_6, Phys. Rev. Lett. **116**, 046403 (2016).
[14] H. K. Pal, F. Piéchon, J.-N. Fuchs, M. Goerbig, and G. Montambaux, Chemical potential asymmetry and quantum oscillations in insulators, Phys. Rev. B **94**, 125140 (2016).
[15] P. Ram and B. Kumar, Theory of quantum oscillations of magnetization in Kondo insulators, Phys. Rev. B **96**, 075115 (2017).
[16] I. Sodemann, D. Chowdhury, and T. Senthil, Quantum oscillations in insulators with neutral Fermi surfaces, Phys. Rev. B **97**, 045152 (2018).
[17] P. Ram and B. Kumar, Inversion and magnetic quantum oscillations in the symmetric periodic Anderson model, Phys. Rev. B **99**, 235130 (2019).
[18] R. Peters, T. Yoshida, and N. Kawakami, Quantum oscillations in strongly correlated topological Kondo insulators, Phys. Rev. B **100**, 085124 (2019).
[19] Y. Tada, Cyclotron resonance in kondo insulator, Phys. Rev. Res. **2**, 023194 (2020).
[20] T. Devakul, Y. H. Kwan, S. L. Sondhi, and S. A. Parameswaran, Quantum Oscillations in the Zeroth Landau Level: Serpentine Landau Fan and the Chiral Anomaly, Phys. Rev. Lett. **127**, 116602 (2021).
[21] B. Kumar, Canonical representation for electrons and its application to the Hubbard model, Phys. Rev. B **77**, 205115 (2008).
[22] S. Sachdev and R. N. Bhatt, Bond-operator representation of quantum spins: Mean-field theory of frustrated quantum Heisenberg antiferromagnets, Phys. Rev. B **41**, 9323 (1990).
[23] R. Kumar and B. Kumar, Fourfold degenerate columnar-dimer ground state in square lattice antiferromagnets, Phys. Rev. B **77**, 144413 (2008).
[24] The zero temperature t_c on a simple cubic lattice from the series expansion method is 0.5 [27], and it is 0.55 from a bond-operator mean-field theory [28].
[25] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders College Publishing, Philadelphia, 1976), Chap. 34, p. 746.
[26] I. M. Lifshitz and A. M. Kosevich, Theory of magnetic susceptibility in metals at low temperatures, Sov. Phys. JETP **2**, 636 (1956).
[27] Z.-P. Shi, R. R. P. Singh, M. P. Gelfand, and Z. Wang, Phase transitions in the symmetric Kondo-lattice model in two and three dimensions, Phys. Rev. B **51**, 15630 (1995).
[28] C. Jurecka and W. Brenig, Bond-operator mean-field theory of the half-filled Kondo lattice model, Phys. Rev. B **64**, 092406 (2001).