Inversion and magnetic quantum oscillations in symmetric periodic Anderson model

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We study symmetric periodic Anderson model of the conduction electrons hybridized with the localized correlated electrons on square lattice. Using the canonical representation of electrons by Kumar, we derive a self-consistent theory of its effective charge and spin dynamics, which produces an insulating ground state that undergoes continuous transition from the Kondo singlet to Néel antiferromagnetic phase with decreasing hybridization, and discovers two inversion transitions for the charge quasiparticles. With suitably inverted quasiparticle bands for moderate to weaker effective Kondo couplings, this effective charge dynamics in the magnetic field coupled to electronic motion produces magnetic quantum oscillations with frequency corresponding to the half Brillouin zone.

I. INTRODUCTION

The magnetic quantum oscillations periodic in inverse magnetic field, namely the de Haas-van Alphen (dHvA) effect [1], were long held to be an exclusive property of the metals, and have provided the direct means to measure the Fermi surfaces thereof (as noted by Onsager [2]). The recent discovery of dHvA oscillations in SmB$_6$, a Kondo insulator, challenges this conventional view [3, 4]. It has forced us to reexamine the physics of Kondo insulators, and reconsider the dHvA effect. The origin of dHvA oscillations in insulators (Kondo or otherwise) is a vigorously pursued problem, with a growing number of theoretical studies and some interesting proposals [5–13].

The Kondo insulators are a subclass of heavy-fermion systems [14, 15], of which the compounds SmB$_6$ [16], YbB$_{12}$ [17], Ce$_3$Bi$_4$Pt$_3$ [18] are some of the best known examples. They behave as paramagnetic insulators (with small gap) at sufficiently low temperatures. But at high temperatures, they are Curie-Weiss metals. The basic setting of Kondo insulators involves the localized $f$ electrons in hybridization with the conduction electrons. The minimal model that applies to heavy-fermion systems is the periodic Anderson model (PAM) with local repulsion, $U$, for the $f$ electrons and the hybridization, $V$, between the $f$ and the conduction electrons [15, 19, 20]. At half-filling, the PAM describes the Kondo insulators.

To exactly realize half-filling, it is common to consider the particle-hole symmetric PAM with nearest-neighbor conduction electron hopping, $t$, on bipartite lattices [21–24]. The Hamiltonian of this symmetric periodic Anderson model (SPAM) can be written as:

$$\hat{H} = -t \sum_{\mathbf{r},\delta} \sum_{s=\uparrow,\downarrow} \hat{c}_{\mathbf{r},s} \hat{c}_{\mathbf{r}+\delta,s} - V \sum_{\mathbf{r}} \sum_{s=\uparrow,\downarrow} \left[ \hat{c}_{\mathbf{r},s}^{\dagger} \hat{f}_{\mathbf{r},s} + \text{h.c.} \right]$$

$$+ U \sum_{\mathbf{r}} \left( \hat{n}_{\mathbf{r},\uparrow} - \frac{1}{2} \right) \left( \hat{n}_{\mathbf{r},\downarrow} - \frac{1}{2} \right)$$

(1)

where $\mathbf{r}$ is summed over the lattice sites, $\delta$ denotes the nearest-neighbors of $\mathbf{r}$, the fermion operators $\hat{c}_{\mathbf{r},s}$ ($\hat{c}_{\mathbf{r},s}^{\dagger}$) create (annihilate) the conduction electrons, $\hat{f}_{\mathbf{r},s}^{\dagger}$ ($\hat{f}_{\mathbf{r},s}$) do likewise for the localized electrons, and $\hat{n}_{\mathbf{r},s} = \hat{n}_{\mathbf{r},s}^{\dagger} \hat{n}_{\mathbf{r},s}$.

In continuation of our study on Kondo insulators [10], motivated by the observation of quantum oscillations in SmB$_6$, we in this paper investigate the dHvA oscillations in the ground state of SPAM. The theory of Kondo insulators, as developed by us for the Kondo lattice model (KLM) in Ref. 10, is applied here to study the orbital response of SPAM to uniform magnetic field. Notably, with this theory of SPAM in the representation of electrons by Kumar [29], we discover two inversion transitions, one each for the charge quasiparticles with narrow and broad dispersions, as $V$ decreases for a given $U$. As we had found for KLM, here too, the quasiparticle band inversion is the key for the dHvA oscillations to occur or not occur. Hence, for strong Kondo couplings ($\sim V^2/U$), we see no dHvA oscillations. But in the regime of intermediate to weaker Kondo couplings, with sufficiently inverted quasiparticle bands, we get clear dHvA oscillations in the insulating ground state of SPAM both in the Kondo singlet and ordered antiferromagnetic (AFM) phases. Akin to what we got for the half-filled KLM, the frequency of these oscillations corresponds to the half Brillouin zone.

This paper is organized as follows. In Sec. II, we formulate a self-consistent theory of the spin and charge dynamics of SPAM. Using this self-consistent theory, in Sec. III, we describe the magnetic quantum phase transition from the Kondo singlet to Néel AFM phase. We then describe the properties of the charge quasiparticles in Sec. IV, and in particular, we discuss the inversion of their dispersions with decreasing $V$, for a fixed $U$. Through this effective charge dynamics, in the Peierls-coupled uniform magnetic field, we investigate and obtain the dHvA oscillations in the insulating ground state of SPAM in Sec. V. We conclude in Sec. VI with a summary of our key findings.

II. SELF-CONSISTENT THEORY OF CHARGE AND SPIN DYNAMICS

To study the properties of SPAM, we use the following canonical representation for $c$ (conduction) and $f$ (local-
ized) electron operators, as prescribed in Ref. 25, on A and B sublattices of a bipartite lattice. While the present consideration is for any bipartite lattice, but later in this paper, we will work only on square lattices.

| \( r \in A \) sublattice | \( r \in B \) sublattice |
|-----------------|-----------------|
| \( \hat{c}^\dagger \) | \( \hat{c}^\dagger \) |
| \( \hat{c} \) | \( \hat{c} \) |
| \( \hat{f} \) | \( \hat{f} \) |

Here, \( \hat{c} \) describes the effective charge dynamics of the SPAM, and \( \hat{f} \) describes the effective spin dynamics of SPAM. Here, \( \rho \) is the total number of lattice sites and \( z \) is the coordination number. Note that in \( \hat{H}_e \), the \( r \) is summed over the entire lattice, unlike in \( \hat{H}_s \), where it is summed over any one of the two sublattices. The \( \delta \) in both cases is summed over all the \( z \) nearest-neighbours. The real-valued decoupling parameters \( \rho_1, \rho_0, \zeta_1 \) and \( \zeta_2 \) are given by the following expectation values.

\[
\rho_1 = \frac{1}{2L} \sum_{r, \delta} \langle \sigma_r \cdot \sigma_{r \delta} \rangle \quad (6a)
\]

\[
\rho_0 = \frac{1}{L} \sum_r \langle \sigma_r \cdot \tau_r \rangle \quad (6b)
\]

\[
\zeta_1 = \frac{2i}{2L} \sum_{r \in A} \sum_{\delta} \langle \hat{a}_{r \delta} \hat{b}_{r \delta} + \hat{b}_{r \delta} \hat{a}_{r \delta} \rangle \quad (6c)
\]

\[
\zeta_2 = \frac{i}{L} \sum_{r \in A} \sum_{\delta} \langle \hat{a}_{r \delta} \hat{b}_{r \delta} \rangle \quad (6d)
\]

We compute these parameters self-consistently in the ground states of Eqs. (4) and (5). But, in general, Eqs. (6) are also applicable at finite temperatures. We find the ground state of \( \hat{H}_e \) by numerical Bogoliubov diagonalization, and that of \( \hat{H}_s \) by doing tripon analysis in the bond-operator representation [26, 27]. The details of these calculations are given below. Note that, the effective spin dynamics of SPAM is similar to that of KLM [10], except now the effective Kondo interaction, \( V \zeta_2 \), is determined self-consistently. However, the charge dynamics of SPAM is more complex compared to KLM, because it involves the charge fluctuations of both conduction as well as localized electrons.

### A. Effective Charge Dynamics

To diagonalize \( \hat{H}_e \) of Eq. (4), we first rewrite it in terms of the spinless fermion creation and annihilation operators, using the definition of the Majorana operators given below Eq. (2). It then reads as follows:

\[
\hat{H}_e = -\frac{t}{2} \sum_{r, \delta} \left[ \hat{a}^\dagger_{r \delta} \hat{b}_{r \delta} + \hat{a}_{r \delta} \hat{b}^\dagger_{r \delta} \right] + \frac{U L}{4} \quad (7)
\]

where \( \rho_{1 \pm} = (1 \pm \rho_1) \) and \( \rho_{0 \pm} = (1 \pm \rho_0) \). By applying Fourier transformation, \( \hat{a}_{\theta \delta} = \sqrt{\frac{2}{L}} \sum_k e^{i \mathbf{k} \cdot \mathbf{r}} \hat{a}_{\theta, \mathbf{k}} \) and \( \hat{b}_{\theta \delta} = \sqrt{\frac{2}{L}} \sum_k e^{i \mathbf{k} \cdot \mathbf{r}} \hat{b}_{\theta, \mathbf{k}} \) (where \( \theta = c, f \)), we get the fol-
lowing expression for $\hat{H}_c$ in the $k$-space.

$$\hat{H}_c = \sum_k \left\{ \frac{t}{2} |\gamma_k| \left[ \rho_{c,k} \hat{a}_{c,k} \hat{b}_{c,k} + \rho_{c,k} \hat{a}_{c,k}^\dagger \hat{b}_{c,k}^\dagger + \text{h.c.} \right] - \frac{V}{2} \left[ \rho_{c,k} \hat{a}_{c,k} \hat{b}_{c,k} \hat{a}_{c,k}^\dagger \hat{b}_{c,k}^\dagger + \text{h.c.} \right] - \frac{V}{2} \left[ \rho_{c,k} \hat{a}_{c,k} \hat{b}_{c,k} \hat{a}_{c,k}^\dagger \hat{b}_{c,k}^\dagger + \text{h.c.} \right] - \frac{U}{2} \left[ \hat{a}_{c,k} \hat{b}_{c,k} - \hat{b}_{c,k} \hat{a}_{c,k}^\dagger \right] \right\}$$

(8)

Here, the Nambu row-vector, $\Psi_k$, is defined as:

$$\Psi_k = \left[ \hat{a}_{c,k}^\dagger \hat{b}_{c,k}^\dagger \hat{b}_{c,k} \hat{a}_{c,k} \right]$$

(9)

and the corresponding column-vector, $\Psi_k^\dagger = \left[ \Psi_k \right]^\dagger$. Moreover, $k \in \text{half-BZ}$, $\gamma_k = \sum_{\delta} e^{i \delta k} = |\gamma_k| e^{i \varphi_k}$, and a gauge transformation, $\hat{a}_{c,k}(k) \rightarrow e^{-i \varphi_k} \hat{a}_{c,k}(k)$, has been applied to absorb the phase $\varphi_k$. The $H_k$ is the following $8 \times 8$ matrix:

$$H_k = \begin{bmatrix} A & 0 \\ -B & -A \end{bmatrix}$$

(10)

with

$$A = -\frac{1}{4} \begin{bmatrix} 0 & t |\gamma_k| \rho_{c,k}^+ & 0 & V \rho_{c,k}^+ \\ t |\gamma_k| \rho_{c,k}^+ & 0 & 0 & V \rho_{c,k}^+ \\ 0 & 0 & 0 & U \\ V \rho_{c,k}^+ & 0 & 0 & 0 \end{bmatrix}$$

and

$$B = -\frac{1}{4} \begin{bmatrix} 0 & -t |\gamma_k| \rho_{c,k}^- & 0 & V \rho_{c,k}^- \\ -t |\gamma_k| \rho_{c,k}^- & 0 & 0 & V \rho_{c,k}^- \\ 0 & 0 & 0 & U \\ -V \rho_{c,k}^- & 0 & 0 & 0 \end{bmatrix}.$$  

(11a, 11b)

We diagonalize Eq. (8) by applying Bogoliubov transformation on $\Psi_k$. To do this, we define a unitary matrix, $U_k$, such that

$$U_k^\dagger H_k U_k = \begin{bmatrix} \varepsilon_k & 0 \\ 0 & -\varepsilon_k \end{bmatrix}$$

(12)

with $\varepsilon_k = \text{DiagonalMatrix}[E_{k,1}, E_{k,2}, E_{k,3}, E_{k,4}]$, and

$$\Psi_k^\dagger U_k = \Lambda_k^\dagger$$

(13)

are the new canonical fermions describing the charge quasiparticles. In terms of these quasiparticle operators, the $H_c$ in the diagonal form reads as:

$$\hat{H}_c = \sum_k \sum_{i=1}^4 E_{k,i} \left( 2 \Lambda_{k,i}^\dagger \Lambda_{k,i} - 1 \right)$$

(14)

where $E_{k,i} > 0$, $i = 1, 2, 3, 4$ are the dispersions of the charge quasiparticles. The ground state of $\hat{H}_c$ is the vacuum of the $\Lambda_{k,i}$ quasiparticles,

$$|0_c\rangle = \prod \left( \prod_i \otimes |0\rangle_{k,i} \right),$$

(15)

with ground state energy per site, $e_{g,c} = -\frac{1}{L} \sum_{k,i} E_{k,i}$.

In order to find the mean-field parameters $\zeta_1$ and $\zeta_2$, we rewrite Eqs. (6d) and (6c) in $k$-space, we first apply the Bogoliubov transformation, $U_k$, and then calculate the expectation values in the ground state of $\hat{H}_c$. This gives us the following equations for $\zeta_1$ and $\zeta_2$.

$$\zeta_1 = \frac{2}{z L} \sum_k |\gamma_k| \langle 0_c | \left( \hat{a}_{c,k}^\dagger \hat{b}_{c,k} - \hat{a}_{c,k} \hat{b}_{c,k}^\dagger \right) + \text{h.c.} | 0_c \rangle$$

(16a)

$$\zeta_2 = \frac{1}{z L} \sum_k \langle 0_c | \Psi_k^\dagger M_{\zeta_1}(k) \Psi_k | 0_c \rangle$$

(16b)

Here, $M_{\zeta_1}(k)$ and $M_{\zeta_2}(k)$ are the following $8 \times 8$ matrices.

$$M_{\zeta_1}(k) = \begin{bmatrix} 0 & -|\gamma_k| & 0 & 0 & 0 & 0 & 0 & 0 \\ -|\gamma_k| & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & |\gamma_k| & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & |\gamma_k| & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

(17)

$$M_{\zeta_2}(k) = \begin{bmatrix} 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

(18)

We know that $\Psi_k^\dagger U_k = \Lambda_k^\dagger$ and $U_k$ is unitary, therefore, $\Psi_k^\dagger = \Lambda_k^\dagger U_k^\dagger$ and $\Psi_k = U_k \Lambda_k$. Moreover, in the ground state, $\langle 0_c | \Lambda_{k,i} \Lambda_{k,j}^\dagger | 0_c \rangle = 0$ and $\langle 0_c | \Lambda_{k,i} \Lambda_{k,j}^\dagger | 0_c \rangle = \delta_{i,j}$. Using these relations in Eqs. (16), we arrive at the final expressions for $\zeta_1$ and $\zeta_2$ that are used to make actual numerical computation.

$$\zeta_1 = \frac{1}{z L} \sum_k \sum_{i=1}^4 |M_{\zeta_1}(k)|_{i+4,i+4}$$

(19a)

$$\zeta_2 = \frac{1}{z L} \sum_k \sum_{i=1}^4 |M_{\zeta_2}(k)|_{i+4,i+4}$$

(19b)
Here, \( \tilde{M}_{(\alpha)}(k) = \mathcal{U}_k M_{(\alpha)}(k) \mathcal{U}_k \).

**B. Effective Spin Dynamics**

We study the spin dynamics of SPAM, given by \( \tilde{H}_s \) of Eq. (3), by doing bond-operator mean-field theory, as we did in Ref. 10 for the KLM. Since every lattice site has a pair of spin-1/2 operators, \( \sigma_r \) and \( \tau_r \), we can use the bosonic bond-operators, \( s_r \) and \( t_r \), corresponding respectively to the local singlet and triplet states with a physical constraint: \( \hat{s}_r^\dagger \hat{s}_r + \sum_{\alpha} \hat{t}_r^\dagger \hat{t}_r = 1 \), to describe the two sets of spin-1/2 operators as [26]:

\[
\sigma_r^\alpha = (\hat{s}_r^\dagger \hat{t}_r + \text{h.c.}) - i \epsilon_{\alpha\beta\gamma} \hat{t}_{r\beta}^\dagger \hat{t}_{r\gamma}
\]

\[
\tau_r^\alpha = - (\hat{s}_r^\dagger \hat{t}_r + \text{h.c.}) - i \epsilon_{\alpha\beta\gamma} \hat{t}_{r\beta}^\dagger \hat{t}_{r\gamma}
\]

where \( \alpha = x, y, z \) denote the three components (and likewise, \( \beta \) and \( \gamma \)) and \( \epsilon_{\alpha\beta\gamma} \) is the Levi-Cevita tensor.

Since the effective Kondo interaction, \( V_{C2} \), would like to form the local singlet between \( \sigma_r \) and \( \tau_r \), we formulate a mean-field theory of \( \tilde{H}_s \) with respect to the Kondo singlet state. In this theory, the reference Kondo singlet state is described by the mean singlet amplitude: \( \langle \hat{s}_r \rangle \approx \bar{s} \), while the triplet fluctuations on top of it are treated quantum mechanically. Thus, we approximate Eqs. (20) as: \( \sigma_r^\alpha \approx \bar{s} (\hat{t}_r + \hat{t}_r^\dagger) \approx - \tau_r^\alpha \), where the interaction between the triplet excitations (triplons) is also neglected. In this theory, the exchange interaction between \( \sigma_r \) and \( \tau_r \) is written as: \( \sigma_r \cdot \tau_r \approx - 3 \bar{s} + \sum_{\alpha} \hat{t}_r^\dagger \hat{t}_r \).

After making all these approximations, the \( \tilde{H}_s \) takes the following mean-field form:

\[
\tilde{H}_s = \frac{t_1 \bar{s}}{4} \sum_{r,\delta,\alpha} (\hat{t}_{r\alpha}^\dagger + \hat{t}_{r\alpha}) (\hat{t}_{r+\delta,\alpha}^\dagger + \hat{t}_{r+\delta,\alpha})
\]

\[
+ \frac{V_{C2}}{2} \sum_r \left( -3 \bar{s}^2 + \sum_{\alpha} \hat{t}_r^\dagger \hat{t}_r - 1 \right)
\]

where the Lagrange multiplier, \( \lambda \), is introduced to satisfy the constraint on average. Under Fourier transformation, \( \hat{t}_r \rightarrow \frac{1}{\sqrt{L}} \sum_k e^{ikr} \hat{t}_{kr} \), it changes to:

\[
\tilde{H}_s = \frac{1}{2} \sum_{k,\alpha} \left\{ \left[ \lambda + \frac{t_1 \bar{s}^2}{2} \right] \left( \hat{t}_{kr}^\dagger \hat{t}_{kr} + \hat{t}_{-kr}^\dagger \hat{t}_{-kr} \right) \right\} + e_0 L
\]

for \( \theta_k = \frac{1}{2} \tanh^{-1} \left[ \frac{t_1 \bar{s}^2 \gamma_k}{t \lambda + t_1 \bar{s}^2 \gamma_k} \right] \). The \( \hat{t}_{kr} \)'s are the new bosonic operators describing triplon quasiparticles with dispersion, \( \varepsilon_k = \sqrt{\lambda (\lambda + t_1 \bar{s}^2 \gamma_k)} \geq 0 \), in term of which the diagonalized \( \tilde{H}_s \) reads as follows.

\[
\tilde{H}_s = e_0 L + \sum_{k,\alpha} \varepsilon_k \left( \hat{t}_{kr}^\dagger \hat{t}_{kr} + \frac{1}{2} \right)
\]

Its ground state energy per site is given as: \( e_{g,s}[\lambda, \bar{s}^2] = e_0 + \frac{3 t_1 \bar{s}^2}{4L} \sum_{k} \varepsilon_k \). Minimizing \( e_{g,s} \) with respect to \( \lambda \) and \( \bar{s}^2 \) gives the following equations whose solution determines \( \lambda \) and \( \bar{s}^2 \), from which the decoupling parameters for the spin part can be obtained as: \( \rho_1 = 1 - 4 \bar{s}^2 \) and \( \rho_1 = 4 \bar{s}^2 (2V_{C2} - \lambda) / 2 \bar{s} \).

We determine \( \zeta_1, \zeta_2, \rho_0 \) and \( \rho_1 \) defined in Eqs. (6) by numerically solving the Eqs. (19) and (25). In the following sections, we discuss the physical behaviour of SPAM obtained from this self-consistent theory.

**III. MAGNETIC TRANSITION IN THE GROUND STATE**

We investigate the ground state properties of SPAM by self-consistently solving Eqs. (19) and (25). In our calculations, we put \( t = 1 \), and compute the parameters of the effective charge and spin dynamics as a function of \( V \) for different values of \( U \). The data obtained on square lattice is plotted in Fig. 1. Notably, for large values of \( V \), we get \( \bar{s}^2 \rightarrow 1 \) and \( \rho_0 \rightarrow -3 \), which correctly implies a perfect Kondo singlet state. However, as \( V \) decreases, \( \bar{s}^2 \) also decreases, and at a \( U \) dependent critical point, \( V_c \), the Kondo singlet phase undergoes a continuous transition to the Néel AFM phase. To this end, we calculate the triplon dispersion, and follow the spin gap in the \( U \)-\( V \) plane to generate the quantum phase diagram. We also compute the charge quasiparticle dispersions, which show the ground state to be insulating, and display two inversion transitions. But first, we discuss the magnetic transition in the ground state.

**A. Triplon dispersion and spin gap**

We compute the triplon dispersion, \( \varepsilon_k \), as given in Eq. (24). It is found to have an energy gap for large values of \( V \) for any \( U \). It remains gapped with decreasing \( V \) up to a critical value, \( V_c \). Thus, for \( V > V_c \), the system is in the spin-gapped Kondo singlet phase. At \( V_c \), however, the \( \varepsilon_k \) becomes gapless at \( k = Q = (\pi, \pi) \), and stays gapless for \( V < V_c \). The gapless nature of \( \varepsilon_k \) at \( Q \)
FIG. 1. The mean-field parameters, $\zeta_1$, $\zeta_2$, $\rho_0$, $\rho_1$, $\lambda$ and $s^2$, of the charge and spin dynamics on square lattice, as a function of $V$ for $U = 4, 6$ and $8$ (with same legend for all three plots). For large $V$, we get $s^2 \rightarrow 1$ and $\rho_0 \rightarrow -3$, which implies a perfect Kondo singlet.

implies Bose condensation of triplons, which in turn implies Néel antiferromagnetic order. This phase transition by decreasing $V$ occurs for any $U$, but at a $V_c$ which depends upon $U$. In Fig. 2, we have plotted the the triplon dispersion obtained from our self-consistent calculations for two different values of $V$ on both sides of $V_c$ for $U = 4$.

From the triplon dispersion, we calculate the spin gap, $\Delta_s$, as a function of $V$ for different values of $U$. Since, the minimum of $\varepsilon_k$ is always at $Q$, the spin gap is given by equation $\varepsilon_Q = \Delta_s$. That is, $\Delta_s = \sqrt{\lambda - zt(z\zeta_1 s^2)}$. The calculated spin gap, plotted in Fig. 3, vanishes continuously at $V_c$, which implies a continuous phase transition in the ground state. We observe that as $U$ is increased, $V_c$ also increases. Hence, the $U$ in SPAM supports the AFM order, while the $V$ favours the Kondo singlet.

B. Quantum phase diagram

We obtain the phase boundary between the Kondo singlet and the Néel AFM phases in the $U$-$V$ plane by the condition, $\varepsilon_Q = 0$, which marks the instability of the Kondo singlet phase towards magnetic ordering. It fixes $\lambda$ of the bond-operator mean-field theory as: $\lambda = zt(z\zeta_1 s^2)$. With this value of $\lambda$, after a few steps of manipulation

FIG. 2. Triplon dispersion, $\varepsilon_k$, in the Brillouin zone of square lattice, in Kondo singlet (blue dashed curve) and AFM phases (red solid curve) at $U = 4$. It is gapped for $V > V_c$, and gapless for $V < V_c$, where $V_c$ marks the onset of gaplessness.

FIG. 3. The spin gap, $\Delta_s$ vs. $V$ for $U = 4, 6$ and $8$, on square lattice. The $\Delta_s$ vanishes continuously as $V$ approaches the critical point, $V_c$, implying a continuous transition from the gapped (Kondo singlet) to the gapless (AFM) phase in the ground state. We also see that when $U$ is increased, $V_c$ too increases, which means that $U$ helps to from the AFM order.
of Eqs. (25) that apply to the gapped phase, we get the following equation for the critical hybridization.

$$V_c = \frac{1}{2} z t (s^2 + 3 y) \left( \frac{\zeta_1}{\zeta_2} \right)$$

(26)

The self-consistent parameters of the spin part are found to become constants at the phase boundary. They are $\rho_0 = 1 - 4 s^2$, $\rho_1 = 12 s^2 y$ and $s^2 = 5/2 - 3 x$, where

$$x = \frac{1}{4L} \sum_k \frac{2 + (\gamma_k/z)}{\sqrt{1 + (\gamma_k/z)}}$$

and

$$y = \frac{1}{4L} \sum_k \frac{(\gamma_k/z)}{\sqrt{1 + (\gamma_k/z)}}$$

are two constants. So, the critical hybridization, $V_c$, depends implicitly upon $U$ through the parameters $\zeta_1$ and $\zeta_2$ of the charge part.

We calculate $V_c$ as a function of $U$ in the ground state by solving Eq. (26) together with Eqs. (19) and (25). It gives us the phase boundary between the quantum paramagnetic Kondo singlet phase and the Néel ordered antiferromagnetic phase in the $U$-$V$ plane. The resulting quantum phase diagram is shown in Fig. 4. We see that the $V_c$ increases with $U$. This is consistent with the fact that the effective Kondo exchange interaction in SPAM is $J \sim V^2/U$ [28, 29]. So, an increase in $U$ reduces the strength of the effective Kondo coupling that allows the AFM order to survive up to the correspondingly larger value of $V_c$. From moderate to large values of $U$, our theory produces a phase boundary that is in qualitative agreement with quantum monte carlo calculations [23]. However, for small $U$’s, the mean-field theory with Néel order is known to give a $V_c$ that rapidly vanishes as $U$ goes to zero [30], whereas the $V_c$ from our calculations tends to a non-zero value even when $U$ becomes zero. It may be emphasized here that our theory, by construction, is better suited for larger values of $U$.

IV. INVERSION TRANSITIONS FOR THE CHARGE QUASIPARTICLES

Now let us discuss the nature of charge quasiparticles in our theory of SPAM. To this end, we compute the dispersions, $E_{k,i}$ (for $i = 1, 2, 3, 4$), of the charge quasiparticles, as defined in Eq. (14). These $E_{k,i}$’s are the positive eigenvalues of the Hermitian matrix $H_k$ of Eq. (10). The evolution of the charge quasiparticle dispersions with $V$ on square lattice is presented in Fig. 5. Note that, for any non-zero $V$, the pair of quasiparticle bands $E_{k,1}$ and $E_{k,2}$ is always lower by a finite energy compared to the pair $E_{k,3}$ and $E_{k,4}$. Since the lowest dispersion, $E_{k,1}$, is strictly $> 0$ for any $V \neq 0$, it describes a state with a non-zero charge gap, that is, an insulating state.

The bands $E_{k,1}$ and $E_{k,2}$ touch each other on the contour $|\gamma_k| = 0$, which in the plots in Fig. 5 is the middle branch from $(\pi, 0)$ to $(\pi/2, \pi/2)$ lying on the boundary of the half-BZ of square lattice. The higher energy bands, $E_{k,3}$ and $E_{k,4}$, also touch each other at $|\gamma_k| = 0$. For large values of $V$, we find the band $E_{k,1}$ ($E_{k,2}$) to have minima (maxima) at $k = (0, 0)$ and maxima (minima) at $k = (0, 0)$. Thus, they are mutually oppositely curved. Likewise, the bands $E_{k,3}$ ($E_{k,4}$) look the same. Notably, $E_{k,3}$ and $E_{k,4}$ are very narrow compared to $E_{k,1}$ and $E_{k,2}$, for large $V$’s, which however become broader with decreasing $V$. Eventually, for sufficiently small values of $V$, they all become of comparable bandwidths.

More importantly, by decreasing $V$, we see two inversion transitions, happening separately for one narrow and one broad quasiparticle band. We note that for $V$ below a characteristic value, $V_{i3}$, the $k = (0, 0)$ is no more the point of minimum for $E_{k,3}$. Instead, for $V < V_{i3}$, the $\Gamma$ becomes a point of local maxima, and the minimum value of $E_{k,3}$ now shifts onto a contour around it. Take a careful look from top to bottom of the second column of plots in Fig. 5. All this while, the $E_{k,4}$ shows no such change. Neither $E_{k,1}$ and $E_{k,2}$ show any qualitative change across $V_{i3}$, but only for a while! As we take $V$ further down, there comes a second special point, $V_{i1}$, at which $E_{k,1}$ (the lowest energy band) starts inverting in the same way by shifting its minimum away from the $\Gamma$ point. See carefully from top to bottom of the first column of plots in Fig. 5. Finally, when $V$ is sufficiently below the inversion point, $V_{i1}$, both $E_{k,1}$ and $E_{k,3}$ get fully inverted and look pretty much like their respective partner bands, $E_{k,2}$ and $E_{k,4}$. Hence, as we found for KLM in Ref. 10, the charge quasiparticle bands of SPAM also undergo inversion transition. But the inversion in SPAM is richer by two! That is, the SPAM exhibits two inversion transitions, first for a (narrow) higher energy charge quasiparticle band, and then for the broad lowest energy charge quasiparticle band. This is indeed a novel finding for the symmetric periodic Anderson model. Figure 6 shows the inversion transition lines corresponding to $V_{i1}$ and $V_{i3}$ from our calculations, together with the phase boundary, in the $U$-$V$ plane.

In Fig. 7, we plot the charge gap, $\Delta_c$, calculated as
FIG. 5. Evolution of the charge quasiparticle dispersions with respect to $V$ (indicated in the third column) on square lattice. The dispersions, $E_{k,i}$ for $i = 1, 2, 3, 4$, are plotted along the high symmetric lines in the half Brillouin zone. We see inversion happening for $E_{k,1}$ (first column; below $V_{1} = 0.96$) and $E_{k,3}$ (second column; below $V_{3} = 2.41$), as $V$ decreases. In the third column, all four bands are plotted together. Note that the higher energy narrow bands tend to become broader as $V$ decreases.

a function of $U/V^2$ (inverse of the effective Kondo coupling) for three different fixed values of $U$. For strong hy-
V. QUANTUM OSCILLATIONS OF MAGNETIZATION

Our experience with KLM shows that, with inverted charge quasiparticle bands, the magnetic quantum oscillations show up nicely even in the insulating state. Since we do find the inversion to occur also for the charge quasi-particles of SPAM, we are confident of seeing dHvA oscillation here too. Thus motivated, we investigate the quantum oscillations of magnetization in the ground state of SPAM. For this purpose, we study the orbital response of Eq. (1) with Peierls coupling to the uniform magnetic field, $B$, via the hopping term which now carries a phase factor involving the vector potential, $A$, and reads as:

$$-i \sum_{\mathbf{r}, \mathbf{s}} e^{i \mathbf{r} \cdot \mathbf{s}} A(x) \delta_{\mathbf{r}, \mathbf{s} + \mathbf{\delta}}.$$  

We take $A = -B y \hat{x}$, for the magnetic field along $\hat{z}$ direction. By rewriting the SPAM with Peierls coupling in the representation of Eq. (2), we derive the following minimal effective model of the field dependent charge dynamics.

$$\hat{H}_{e}^{[B]} = -\frac{i t}{2} \sum_{\mathbf{r} \in A} \sum_{\mathbf{\delta}} \left\{ \cos(2\pi \alpha e y \mathbf{\delta} \cdot \mathbf{\delta}) \left[ \tilde{\psi}_{a, \mathbf{r}} \tilde{\phi}_{a, \mathbf{r} + \mathbf{\delta}} + \rho_1 \tilde{\phi}_{b, \mathbf{r} + \mathbf{\delta}} \tilde{\phi}_{a, \mathbf{r}} \right] \right\} - \frac{i V}{2} \sum_{\mathbf{r} \in A} \left[ \tilde{\psi}_{a, \mathbf{r}} \tilde{\phi}_{a, \mathbf{r}} + \rho_0 \tilde{\phi}_{b, \mathbf{r}} \right] - \frac{U}{2} \sum_{\mathbf{r} \in B} \left[ \hat{a}^\dagger_{\mathbf{r}} \hat{a}_{\mathbf{r}} + \sum_{\mathbf{r} \in B} \hat{b}^\dagger_{\mathbf{r}} \hat{b}_{\mathbf{r}} \right] (27)$$

This is very similar to what we obtained for the KLM [10]. Here, $\alpha = eB a^2/h$ is the reduced magnetic flux, with $a$ as the lattice constant. The $\mathbf{r}_y$ and $\mathbf{\delta} = \mathbf{\delta}/|\mathbf{\delta}|$ are the $y$ coordinate of $\mathbf{r}$ and unit vector for $\mathbf{\delta}$, respectively. For $\alpha = 0$, Eq. (27) would reduce to Eq. (4).

To calculate the magnetization, $M$, versus $B$ from this Hofstadter like problem, we put zero field values of $\rho_0$ and $\rho_1$ (as in Fig. 1) in Eq. (27), and numerically compute its ground state energy per site, $e_g$, as a function of $\alpha = p/q$ for integer $p = 1, 2, \ldots, q$ with $q = 601$ (a prime number) on square lattice. Using the definition: $M = -\partial e_g/\partial \alpha$, we calculate $M$ as a function of $\alpha$.

In Fig. 8, we present the data from this calculation for a fixed $U = 4$ and different $V$’s. Note that for $U = 4$, the critical point is $V_c \approx 0.7$, and the inversion points are $V_{i1} = 0.96$ and $V_{i3} = 2.41$. Thus, in Fig. 8, by varying $V$, we are going across the critical point from the Kondo singlet into the Néel phase, with inverted quasiparticle bands. This data shows that the dHvA oscillations become more prominent with decreasing $V$, that is, as the effective Kondo coupling gets weaker. Thus, we do get dHvA oscillations in the Kondo singlet phase close to critical point, but they are less prominent compared to the oscillations in the AFM phase. Moreover, for $V > V_{i3}$, we find the dHvA oscillations to be completely absent. In the range $V_{i1} < V < V_{i3}$, but close to $V_{i1}$, we begin to see very faint oscillations, which are not plotted here.

May be for very large system sizes, one could also resolve such weak oscillations. These findings in the insulating ground state of SPAM clearly reaffirm that the inversion of charge quasiparticle bands is very important for the occurrence of dHvA oscillations in Kondo insulators.

By doing Fourier transformation of the $M/\alpha$ vs $1/\alpha$ data in Fig. 8(b), we find the dominant frequency of
dHvA oscillations to be \( \nu_0 = 0.5 \). It corresponds to the area enclosed by the contour, \(|\mathbf{k}| = 0\), that is, the half Brillouin zone of the square lattice. Recall the relation, \( A = (2\pi/a)^2 \nu \), between the area \( A \) of an extremal orbit perpendicular to magnetic field on a constant energy surface in \( k \)-space and the frequency \( \nu \) (in units of \( \hbar / e a^2 \)) of the dHvA oscillations. All these findings for SPAM are fully consistent with what we had obtained for KLM [10].

In Fig. 9, we present the quantum oscillation data for a fixed \( V = 0.6 \) and different \( U \)’s. In this case, the system goes into the Néel phase for \( U > 2.45 \), and the inversion occurs for \( U > 1.59 \). This data leads to the same conclusions as drawn above. That is, the amplitude of dHvA oscillations grows by decreasing effective Kondo coupling (by increasing \( U \) here), the dominant oscillation frequency, \( \nu_0 = 0.5 \), corresponds to the area enclosed by the \(|\mathbf{k}| = 0 \) contour (half Brillouin zone on square lattice), and the inversion of charge quasiparticle bands is necessary for the dHvA oscillations to occur.

**FIG. 8.** The dHvA oscillations in the insulating ground state of the symmetric periodic Anderson model on square lattice, for \( V = 0.75, 0.72, 0.7 \) (Kondo singlet) and \( V = 0.65, 0.6, 0.5 \) (Néel AFM) for \( U = 4 \). The legend of plot (a) also applies to (b) and (c). We see clear oscillations, both in the Kondo singlet and AFM phases, whose amplitude grows by decreasing \( V \). The dominant frequency, \( \nu_0 = 0.5 \), corresponds to the half-Brillouin zone, i.e., the area enclosed by \(|\mathbf{k}| = 0 \) contour.

**FIG. 9.** The dHvA oscillations in the insulating ground state of the symmetric periodic Anderson model on square lattice for \( U = 2.42, 2.44 \) (Kondo singlet) and \( U = 3, 4, 5, 6 \) (Néel AFM) for \( V = 0.6 \).
VI. CONCLUSION

In this paper, we have studied the SPAM (symmetric periodic Anderson model) on square lattice, using the theory of Kondo insulators that we first developed for the half-filled KLM (Kondo lattice model) in Ref. 10. Our approach appropriately produces the basic features of the insulating ground state of the SPAM. More importantly, it discovers the inversion phenomena for the charge quasiparticles of SPAM, similar to what we had found for KLM. In fact, here, we get two inversion transitions (by decreasing $V$ for a fixed $U$), first for a narrow higher energy band and then for the lowest energy broad band of the charge quasiparticles. In response to the uniform magnetic field coupled to the electronic motion, our calculations produce dHvA oscillations of the frequency corresponding to the half Brillouin zone. The direct bearing of inversion on quantum oscillations is clearly affirmed by the fact that the dHvA oscillations appear only after the charge quasiparticle bands have suitably inverted. Thus, our theory produces a consistent physical picture of the inversion and magnetic quantum oscillations in both the conventional models of Kondo insulators, viz, the half-filled Kondo lattice model and the symmetric periodic Anderson model.

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