Kondo Effect of a Magnetic Ion Vibrating in a Harmonic Potential

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To discuss Kondo effects of a magnetic ion vibrating in the sea of conduction electrons, a generalized Anderson model is derived. The model includes a new channel of hybridization associated with phonon emission or absorption. In the simplest case of the localized electron orbital with the s-wave symmetry, hybridization with p-waves becomes possible. Interesting interplay among the conventional s-wave Kondo effect and the p-wave one and the Yu-Anderson type Kondo effect is found and the ground state phase diagram is determined by using the numerical renormalization group method. Two different types of stable fixed points are identified and the two-channel Kondo fixed points are generically realized on the boundary.

KEYWORDS: Kondo effect, impurity Anderson model, electron-phonon coupling, numerical renormalization group, two-channel Kondo effect

1. Introduction

Recently, a new type of ionic structure, a network of cages filled or unfilled by guest ions, has attracted much interest in the research area of condensed matter physics. When the radius of filled ion is smaller than the size of cage, the guest ions vibrate with large amplitude but almost without effect of interference with oscillations of the ions in the neighboring cages. It is expected that various unusual phenomena are possible due to such incoherent vibrations. Typical examples of this class of materials are β-pyrochlore oxides AO\textsubscript{2}O\textsubscript{6} (A = K, Rb or Cs), filled skutterudites RT\textsubscript{2}X\textsubscript{12} (R = rare earth or alkaline earth; T = Fe, Ru, Pt or Os; X = P, As, Ge or Sb) and type-I clathrate compounds.

The family of β-pyrochlore oxides, especially KO\textsubscript{2}O\textsubscript{6}, is a good example where several qualitatively new phenomena are observed due to the anharmonicity of the cage potential\textsuperscript{1}; concave-downward temperature dependence of resistivity\textsuperscript{2}, peak structure of NMR relaxation rate at potassium site at low temperatures\textsuperscript{3}, occurrence of superconductivity\textsuperscript{4} and the structural phase transition which takes place below the superconducting transition temperature.\textsuperscript{2} Concerning the resistivity and the NMR relaxation rate, Dahm and one of the authors considered a simple model for the anharmonic potential which includes the fourth order term of the ion displacement. They have shown that the unusual temperature dependence of these quantities are explained by calculating the retarded phonon propagator within the self-consistent quasi-harmonic approximation.\textsuperscript{5} Detailed properties of the spectral function of the local ion are also investigated for various types of the cage potential including a double-well type.\textsuperscript{5} The more realistic model that the ion vibrates in the three-dimensional cage potential with the third order anharmonic term specific to the tetrahedral symmetry of the β-pyrochlore compounds is discussed by one of the authors and Tsunetsugu.\textsuperscript{7–9} It is shown that the third order anharmonic term has important effect on the superconductivity and is also responsible to the first order structural transition below the superconducting transition temperature.

Another interesting behavior is reported for the filled skutterudite compound, SmOs\textsubscript{4}Sb\textsubscript{12}.\textsuperscript{10–14} It shows a large specific heat coefficient \(\gamma\), which is robust against magnetic fields.\textsuperscript{11} One possible scenario of this behavior is that a non-magnetic Kondo effect is realized by local vibrations of the guest ions.\textsuperscript{15, 16} Motivated by the unusual heavy fermion behaviors of SmOs\textsubscript{4}Sb\textsubscript{12}, we have started a systematic study on the interplay between local electron correlation and electron-phonon coupling.\textsuperscript{17}

Let us review the previous studies related to Kondo effect coupled with local vibrations. To include effects of the local oscillations, two different types of models have been considered, the breathing mode of the cage and the transverse modes of the cage, i.e., the relative displacement between the ion and the cage.

Firstly, a theoretical model of a magnetic ion coupled with the breathing mode is known as Anderson-Holstein model.\textsuperscript{18} In this model the one-electron energy level of the impurity orbital is modified by the amplitude of the breathing mode. By applying Lang-Firsov transformation\textsuperscript{19}, it can be shown that the interaction induces an effectively attractive electron-electron interaction (for example see Ref. 20). If the electron-phonon coupling overcomes Coulomb repulsion, the electronic states of the impurity result in a quasi degenerate doublet, the empty and the doubly occupied states. If there is a matrix element between the doublet, it is possible that the non-magnetic doublet works as a pseudo spin and induces Kondo effect. Actually, a recent study shows that magnetically robust Kondo effect is possible even in relatively high magnetic fields when the effect of anharmonicity of the breathing mode is included.\textsuperscript{21}

Secondly, a model of a non-magnetic ion which oscillates in the sea of conduction electrons was proposed by Yu and Anderson.\textsuperscript{22} In this model, the conduction electrons are scattered by the vibrations of the ion. For simplicity spins of conduction electrons are neglected. Yu and Anderson considered only the first order term of ionic displacement which produced the scattering pro-
cesses between the s-wave conduction electrons to the p-wave ones. It is shown that the resultant effective potential for the ion displacement behaves like a double well potential when the electron-phonon coupling is strong. Therefore a new type of Kondo effect is expected because logarithmic divergence appears when there are doubly degenerate states connected each other through scattering processes of conduction electrons.\textsuperscript{23–25}

This paper is a comprehensive report on the effects of vibration of a magnetic ion coupled with spinful conduction electrons. Some of the results have been published in the previous letter.\textsuperscript{17} In §2 we construct a generalized impurity Anderson model of the magnetic ion. When we ignore spin-orbit interaction, the generalized gradient theorem\textsuperscript{26} enables us to expand hybridization term with respect to the ion displacement. As a result phonon-assisted hybridization is naturally induced in addition to the conventional one. In §3 and §4, we apply the numerical renormalization group (NRG) method\textsuperscript{27,28} to the simplest case, where the impurity ion with an s-wave orbital vibrates in a one-dimensional harmonic potential. From the analysis of energy spectra obtained from the NRG calculations, one can identify three different types of NRG flows at low temperatures which define the low energy fixed points. We obtain the phase diagram characterized by the fixed points in the parameter space of phonon-assisted hybridization and Coulomb interaction. The fixed point analysis is described in detail in the present paper. Various physical quantities which include the spin and charge susceptibilities and the mean square amplitude of the displacement are also discussed. Finally, conclusions and some future problems are summarized in §5.

\section{A generalized impurity Anderson model for a vibrating magnetic ion}

\subsection{Expansion of hybridization term by ion displacement}

In this section we derive a generalized impurity Anderson model for a magnetic ion vibrating in a cage potential. When the ion is static, it has to be equivalent to the usual impurity Anderson model.\textsuperscript{29} It is assumed that the effects of vibrations are taken into account through hybridization modified by the shift of the ionic position. Conduction electrons are assumed to be a non-interacting system and decomposed into the partial waves,

\begin{equation}
H_c = \sum_{k\sigma} \varepsilon(k) c_{k\sigma}^\dagger c_{k\sigma} = \sum_{k\sigma} \sum_{\ell m} \varepsilon(k) c_{\ell m\sigma}^\dagger(k) c_{\ell m\sigma}(k),
\end{equation}

where \(\varepsilon(k)\) is the dispersion relation and \(c_{k\sigma}^\dagger\) (\(c_{k\sigma}\)) is an annihilation (creation) operator of the conduction electrons. \(c_{\ell m\sigma}(k)\) is defined from \(c_{k\sigma}\) using the spherical harmonics \(Y_{\ell m}(\hat{k})\),

\begin{equation}
c_{\ell m\sigma}(k) = \sqrt{4\pi} \sum_k Y_{\ell m}^\ast(\hat{k}) c_{k\sigma},
\end{equation}

The dynamics of the ion with position vector \(Q\) is described by the following Hamiltonian,

\begin{equation}
H_{\text{ion}} = -\frac{\hbar^2}{2M} (\nabla Q)^2 + V_{\text{cage}}(Q),
\end{equation}

where \(V_{\text{cage}}(Q)\) is the cage potential and \(M\) the mass of the ion. Hybridization modified by the ion displacement \(Q\) is expressed by the overlap integral between a plane wave \(1/\sqrt{\Omega} e^{i k r}\) and the localized orbitals of the magnetic ion, where \(\Omega\) is the volume of the system. Without the spin orbit interaction, \(\ell\)-wave electron orbitals, \(\psi_{\ell m}(r) \equiv u_{\ell}(r) Y_{\ell m}(\hat{r})\), satisfy the following Schrödinger equation,

\begin{equation}
\left( -\frac{\hbar^2 \nabla^2}{2m} + V_{\text{nucleus}}(r) - \varepsilon_\ell \right) \psi_{\ell m}(r) = 0,
\end{equation}

where the potential \(V_{\text{nucleus}}(r)\) is assumed to be isotropic and \(m\) is the mass of electron. When the ion is shifted from the origin by \(Q\), the relative coordinate from the ion to electron coordinate \(r\) is given by \(r - Q\). Therefore the overlap integrals are expressed by

\begin{equation}
V_{(k; \ell m)}(Q) = \frac{g}{\sqrt{\Omega}} \int d^3 r e^{-i k r} \psi_{\ell m}(r - Q),
\end{equation}

where \(g\) is a coupling constant. With these integrals, hybridization terms modified by the ion displacement are given as

\begin{equation}
H_{\text{hyb}} = \sum_{k\sigma} \sum_m \{ V_{(k; \ell m)}(Q) c_{k\sigma}^\dagger f_{\ell m\sigma} + \text{h.c.} \},
\end{equation}

where \(f_{\ell m\sigma}\) are the annihilation (creation) operators for the localized \(\ell\)-wave orbitals. We expand the overlap integrals with respect to the ion displacement \(Q\). In this paper we focus on the first order terms of \(Q\). The hybridization terms expanded within \(O(Q)\) are given as

\begin{equation}
H_{\text{hyb}} = \sum_{k m\sigma} \{ V_{\ell} c_{\ell m\sigma}(k) f_{\ell m\sigma} + \frac{1}{q_{1, m'}} \sum_{m' = -1}^{1} q_{1, m'}^* \}
\end{equation}

\begin{equation}
\times \left[ V_{\ell + 1} c_{\ell + 1, m + m' \sigma}(k) f_{\ell m\sigma} + V_{\ell - 1} c_{\ell - 1, m + m' \sigma}(k) f_{\ell m\sigma} + \text{h.c.} \right],
\end{equation}

where \(V_{\ell}, V_{\ell + 1}\) and \(q_{1, m}\) are defined in Appendix. It is obvious that the rotational symmetry \(SO(3)\) is preserved in the generalized hybridization term (2.7).

Under the simplest assumption that the ion has an \(s\)-wave electron orbital, the hybridization terms (2.7) are rewritten based on the Cartesian coordinate system as

\begin{equation}
H_{\text{hyb}} = \sum_{k\sigma} \{ V_{c_{1\sigma}}^\dagger(k) f_{\sigma} + \text{h.c.} \}
\end{equation}

\begin{equation}
+ \sum_{k\sigma} \sum_{i=x, y, z} \{ V_{c_{1, i\sigma}}^\dagger(k) f_{\sigma} q_{i} + \text{h.c.} \},
\end{equation}

where \(c_{1\sigma}\) are the annihilation operators for the \(s\) (\(p_i\))-wave components of the conduction electrons. It is verified easily that \(V_{1}^{(0, 0)} = V_{1}^{(0, \pm 1)} = \nabla\) because of the rotational invariance.
For simplicity, we study the situation that the ion vibrates along one direction, say \( x \)-direction. Using a one-dimensional harmonic potential \( (1/2)M \omega^2 Q^2 \), we get the Hamiltonian for this study,

\[
H = H_c + H_{hyb} + H_{local},
\]

\[
H_c = \sum_{k \sigma} \varepsilon(k) \{ c_{k \sigma}^{\dagger}(k) c_{k \sigma}(k) + c_{k \sigma}^{\dagger}(k) c_{-k \sigma}(k) \},
\]

\[
H_{hyb} = \sum_{k \sigma} \{ V_0 c_{k \sigma}^{\dagger}(k) f_{\sigma} + h.c. \}
+ V_1 c_{1 \sigma}(k) f_{\sigma} (a + a^\dagger) + h.c.,
\]

\[
H_{local} = \hbar \omega a^\dagger a + \varepsilon_f \sum_{\sigma} f_{\sigma}^\dagger f_{\sigma} + U f_{\uparrow}^\dagger f_{\uparrow} f_{\downarrow}^\dagger f_{\downarrow},
\]

where \( \sqrt{7}/\sqrt{2} \) is set to \( V_1 \) and \( a (a^\dagger) \) is the annihilation (creation) operator of the phonon. For the localized electron orbital, the annihilation (creation) operator is expressed by \( f_{\sigma} (f_{\sigma}^\dagger) \) and \( \varepsilon_f \) is its energy given by eq. (2.4) and \( U \) the Coulomb interaction. When we restrict the isotropic degrees of freedom of the ionic vibrations to one particular direction, the SO(3) symmetry is lowered to the discrete inversion symmetry; \( r \to -r \) and \( Q \to -Q \).

### 2.2 Comments on the symmetries

There are three relevant quantum numbers for the present model (2.9)–(2.12). It is obvious that the total electron number \( N_{\text{tot}} \) and the \( z \) component of total spin \( S_z \) are conserved. The last one is related to the inversion symmetry mentioned in the previous section. The operation of the inversion \( \mathcal{P} \) is described in the second-quantized notations,

\[
\mathcal{P} f_{\sigma} \mathcal{P}^{-1} = f_{\sigma}, \tag{2.13}
\]

\[
\mathcal{P} c_{0 \sigma}(k) \mathcal{P}^{-1} = c_{0 \sigma}(k), \tag{2.14}
\]

\[
\mathcal{P} c_{1 \sigma}(k) \mathcal{P}^{-1} = -c_{1 \sigma}(k), \tag{2.15}
\]

\[
\mathcal{P} q \mathcal{P}^{-1} = -q. \tag{2.16}
\]

We characterize the inversion symmetry by the total parity \( \mathcal{P} \) which is defined by the sum between the number of \( p \)-channel conduction electrons \( N_p \) and the number of harmonic phonons \( N_{\text{ph}} \), namely \( \mathcal{P} = N_p + N_{\text{ph}} \equiv 0 \) or \( 1 \) (mod 2).\(^{30}\) This is based on the fact that, within \( O(Q) \), phonon-assisted hopping between the impurity orbital and the \( p \)-channel conduction electrons has to accompany absorption or emission of one phonon. This quantum number plays a crucial role in the analyses of the energy spectra.

In the original model used by Yu and Anderson (YA model),\(^{22}\), it is assumed that a non-magnetic ion, which is trapped in a one-dimensional harmonic potential, vibrates in spinless conduction electrons. The first order process of the displacement induces scattering processes between the \( s \)-wave and \( p \)-wave conduction electrons. No localized electron orbital is introduced in the model. The original YA model is written as

\[
H_{\text{YA}} = \sum_k \{ \varepsilon_0(k) c_0^\dagger(k) c_0(k) + \varepsilon_1(k) c_1^\dagger(k) c_1(k) \}
+ \sum_{k,k'} \{ V_1 c_0^\dagger(k) c_1(k') (a + a^\dagger) + h.c. \}
+ \hbar \omega a^\dagger a, \tag{2.17}
\]

where \( c_0(k) (c_1(k)) \) are the annihilation operators for the spinless \( s \)-wave (\( p \)-wave) conduction electrons with the dispersion relation \( \varepsilon_0(k) (\varepsilon_1(k)) \).

In general, \( \varepsilon_0(k) \) and \( \varepsilon_1(k) \) are different. However if we assume that \( \varepsilon_0(k) \) and \( \varepsilon_1(k) \) are the same, an artificial symmetry comes into existence. The symmetry, which we call channel symmetry, is the invariance under the following transformation \( \mathcal{I} \).

\[
\mathcal{I} c_0(k) \mathcal{I}^{-1} = c_1(k), \tag{2.18}
\]

\[
\mathcal{I} c_1(k) \mathcal{I}^{-1} = c_0(k). \tag{2.19}
\]

With the channel symmetry, the Hamiltonian (2.17) can be decomposed into two detached parts by introducing the bonding and antibonding orbitals,

\[
c_c(k) = \frac{c_0(k) + c_1(k)}{\sqrt{2}}, \tag{2.20}
\]

\[
c_a(k) = \frac{c_0(k) - c_1(k)}{\sqrt{2}}, \tag{2.21}
\]

and there is no matrix element between the two potential minima in contrast to the implicit assumption made by Yu and Anderson. Therefore the breaking of the channel symmetry is needed for the realization of Yu and Anderson type Kondo (YA) effect. Matsura and Miyake showed that potential scattering processes of the second order of the ion displacement play such a role.\(^ {31} \)

These discussions are also valid for the spinful fermion case. As for the present Hamiltonian (2.9), the introduction of the localized impurity orbital serves as a source of breaking of the channel symmetry. Therefore the Hamiltonian (2.9) at \( U = 0 \) is one realization of the YA model extended to the spinful case.

### 3. Numerical renormalization group approach

#### 3.1 Mapping to Wilson chains

It is well known that for the ordinary impurity Anderson model the numerical renormalization group (NRG) method is a powerful one to calculate energy spectra and various physical quantities with high accuracy.\(^ {27, 28} \) We apply the NRG method to the present model by discretizing the two continuous conduction bands in the logarithmic energy scales characterized by \( \Lambda \). Both the \( s \)-wave and \( p \)-wave conduction bands can be discretized in the same way because the dispersion relation \( \varepsilon(k) \) is assumed to have no angular dependence on \( k \). The discretized Hamiltonian is given by the two one-dimensional half-chains corresponding to the \( s \)-wave and \( p \)-wave conduction bands, which may be called Wilson chains,

\[
H_N = \Lambda^{N-1}.
\]
Fig. 1. (Color online) (a) Graphical representation of the Hamiltonian (3.1). The wavy line represents phonon-assisted hopping while the straight lines usual hoppings. (b) The YA model mapped to the Wilson chains.

\[ \begin{align*}
H_{2\text{-site}} &= H_{2\text{-site}}^{(0)} + H_{2\text{-site}}^{(1)} \\
H_{2\text{-site}}^{(0)} &= V_0 \sum_{\sigma} \{ p_{\sigma} f_\sigma + \text{h.c.} \} (a + a^\dagger) \\
&+ \hbar \omega a^\dagger a,
\end{align*} \]  

where \( H_{2\text{-site}}^{(0)} \) and \( H_{2\text{-site}}^{(1)} \) are the contributions from the electron parts of the doublet.

For \( U = 0 \), the two-site Hamiltonian is solved exactly using the canonical transformation called Lang-Firsov transformation,\(^{19}\) \( e^{iS} \) with

\[ S = i\lambda \sum_\sigma (A_\sigma A^{\dagger}_\sigma + B_\sigma B^{\dagger}_\sigma)(a - a^\dagger), \]

where \( A_\sigma \) and \( B_\sigma \) are the annihilation operator for the antibonding and bonding orbitals, \( A_\sigma = (1/\sqrt{2})(f_\sigma - p_{0,\sigma}) \) and \( B_\sigma = (1/\sqrt{2})(f_\sigma + p_{0,\sigma}) \). The coupling constant is given by \( \lambda \equiv -V_1/\hbar \omega \). Then the transformed Hamiltonian is written as

\[ e^{-i S} H_{2\text{-site}}^{(0)} e^{i S} = -\frac{V_0^2}{\hbar \omega} \left( \sum_\sigma (A_\sigma A^{\dagger}_\sigma + B_\sigma B^{\dagger}_\sigma) \right)^2 + \hbar \omega a^\dagger a. \]

We obtain the doubly degenerate ground states |\( L \rangle \) and |\( R \rangle \), which may be called polaron doublet (PD), with the ground-state energy \( E_{\text{PD}} \),

\[ E_{\text{PD}} = -4V_0^2/\hbar \omega. \]

These two degenerate states are characterized by the expectation values of the ionic position \( q \).

\[ \langle L \vert q \rangle L \rangle = -\langle R \vert q \rangle R \rangle = 2\sqrt{2} \lambda, \]

\[ \langle L \vert q^2 \rangle L \rangle = \langle R \vert q^2 \rangle R \rangle = \frac{16\lambda^2 + 1}{2}. \]

One can see that the PD is formed both for spinful and spinless cases and it plays a similar role as the localized spin for the usual spin Kondo effect.

In the following discussion, it is important to note that the electron parts of the doublet are written as

\[ B_\uparrow^\dagger B_\downarrow^\dagger |\text{el}\rangle = |\text{LS}\rangle_{\text{el}}^\uparrow + |\text{PS}\rangle_{\text{el}}^\uparrow, \]

\[ A_\uparrow^\dagger A_\downarrow^\dagger |\text{el}\rangle = |\text{LS}\rangle_{\text{el}}^\downarrow - |\text{PS}\rangle_{\text{el}}^\downarrow, \]

where

\[ |\text{LS}\rangle_{\text{el}} = \frac{f_\uparrow^\dagger f_\downarrow^\dagger + p_{0,\uparrow}^\dagger p_{0,\downarrow}^\dagger}{2} |\text{vac}\rangle_{\text{el}}, \]

represents a local singlet with even parity while

\[ |\text{PS}\rangle_{\text{el}} = \frac{f_\uparrow^\dagger p_{0,\uparrow}^\dagger - f_\downarrow^\dagger p_{0,\downarrow}^\dagger}{2} |\text{vac}\rangle_{\text{el}}, \]

a pair singlet with odd parity. Similarly, the phonon parts of the doublet are written as

\[ |\ell\rangle_{\text{ph}} = |\text{even}\rangle_{\text{ph}}^\uparrow + |\text{odd}\rangle_{\text{ph}}^\uparrow. \]
states and eigenvalues are written as \( U \rangle \). Then within the first order perturbation of \( H^{(1)} \), which we will write as composed of the impurity site connected to the single Wilson chain, where \( \text{even} \rangle \), \( \text{odd} \rangle \), \( | 0 \rangle \), and \( | R \rangle \) are not eigenstates of the total parity, \( P \).

The degeneracy of the PD is lifted by Coulomb interaction \( H^{(1)}_{\text{PD}} \), which may be treated by the perturbation theory. In fact energy shift from \( E_{\text{PD}} \) is obtained by the following eigenvalue equation,

\[
\det \begin{pmatrix} \Delta E_{\text{PD}} - \langle L | H^{(1)}_{\text{PD}} | L \rangle & -\langle L | H^{(1)}_{\text{PD}} | R \rangle \\ -\langle R | H^{(1)}_{\text{PD}} | L \rangle & \Delta E_{\text{PD}} - \langle R | H^{(1)}_{\text{PD}} | R \rangle \end{pmatrix} = 0.
\]

Then within the first order perturbation of \( U \), the eigenstates and eigenvalues are written as

\[
| \pm \rangle = \frac{| L \rangle \pm | R \rangle}{\sqrt{2}},
\]

\[
E^{\pm}_{\text{PD}} = E_{\text{PD}} + \frac{U}{4} \left( 1 \pm e^{-8\lambda^2} \right).
\]

It shows that Coulomb interaction works on the PD like a transversal magnetic field for a localized spin. The energy gap between \( | + \rangle \) and \( | - \rangle \), \( \Delta_{\text{PD}} \equiv (U/2)e^{-8\lambda^2} \), is small when the electron-phonon coupling \( \lambda \) is strong, of the order of unity. Unlike \( | L \rangle \) and \( | R \rangle \), \( | + \rangle \) and \( | - \rangle \) are the eigenstates of the total parity. The parity of \( | + \rangle \) is even \((P = 0)\) and that of \( | - \rangle \) is odd \((P = 1)\).

4. Results of the NRG calculations

4.1 Classification of fixed points from energy spectra

To begin with, we summarize the NRG calculations for the usual impurity Anderson model. After the mapping to a Wilson chain, the discretized Hamiltonian is composed of the impurity site connected to the single semi-infinite Wilson chain, which we will write as \( f \) site and \( s_i \) \((i = 0 \sim n)\) sites. The number of the NRG steps \( n \) corresponds to the energy scale of the system. When \( n \) is sufficiently large, energy flow approaches to the unique low-temperature fixed point.

The stable fixed point corresponds to the unitary limit of Kondo effect. In the limit, the low-energy spectrum is isomorphic to that of the Hamiltonian consisting of two parts, the singlet bond between \( f \) and \( s_0 \) sites and the remaining free Wilson chain from \( s_1 \) to \( s_n \).

Concerning analysis of the fixed point, it is essential to note that the low-energy spectrum depends on even or odd of \( n \). Eigenstates of the Wilson chain are specified by the set of quantum numbers, \([ N^{\text{tot}}, S^{\text{tot}} \] \). For a tight binding Hamiltonian with only off-diagonal matrix elements, single-particle energies are symmetric with respect to positive and negative energies. When \( n \) is odd, the middle one of eigenenergies must be zero. At half-filling Fermi energy should be also zero. Therefore, the ground states have four-fold degeneracy which are specified by the quantum numbers, \([n - 1, 0], [n, \pm \frac{1}{2}] \) and \([n + 1, 0]\). For an even \( n \), there is no eigenvalue at \( E = 0 \) and therefore the ground state is unique with the quantum number \([n, 0] \), see Fig. 2.

Now let us discuss the fixed points for the present model. After \( n \) steps in the NRG, the system consists of \( 2n + 3 \) sites, the localized \( f \) orbital and the two Wilson chains, \( s_0, s_1, \cdots, s_n \) and \( p_0, p_1, \cdots, p_n \). Our numerical results by the NRG method show that there are only two stable fixed points: \( s \)- and \( p \)-type. The \( s \)-type fixed point schematically shown in Fig. 3(a) is characterized by the energy spectrum which is isomorphic to that of the system composed of tightly bound \( f - s_0 \) singlet and two independent Wilson chains whose length is different, \( n \) sites for the \( s \)-chain and \( n + 1 \) sites for the \( p \)-chain. It is important to include the parity as a quantum number, \([N^{\text{tot}}, S^{\text{tot}} \), \( P \]. Concerning the \( s \)-type fixed point the phonon part does not play any important role and the total parity \( P \) is simply determined by the number of electrons in the \( p \)-channel. From Fig. 3(a) it is straightforward to see that the quantum numbers of the degenerate ground states are those given in Table I depending on even or odd \( n \). As an example, we show in Table II a part of the low energy spectra of the \( s \)-type fixed point which correspond to the one particle excited states. The other fixed point defined as \( p \)-type is depicted in Fig. 3(b). The energy spectrum at low energies is isomorphic to that for the system with isolated \( f - p_0 \) singlet bond and two independent Wilson chains, \( n + 1 \) sites for the \( s \)-chain and \( n \) sites for the \( p \)-chain. One important non-trivial fact obtained by the present NRG calculations is that the quantum number for the part of \( f - p_0 \) singlet is always given by \([2, 0, 1]\), odd parity in the same way as the two-site problem discussed in §3.2. Therefore the quantum numbers of the ground states for the entire system are given by those shown in Table I.

![Fig. 2. (Color online) Schematic one-particle energy levels of a single Wilson chain with (a) an odd number of sites and (b) an even number of sites.](image)

![Fig. 3. (Color online) Graphical representations of the two types of the energy spectra.](image)
Lastly, we discuss the unstable fixed points which separate the regions of the $s$- and $p$-type fixed points. Here, we briefly review the $2$-channel Kondo model. The model consists of a local moment coupled antiferromagnetically with two types of conduction electrons.\cite{32,33,34} The NRG calculations show that $2$-channel Kondo effect is realized when the two antiferromagnetic coupling constants, $J_a$ and $J_b$, are perfectly equal.\cite{33} The energy spectra obtained from the NRG calculations are summarized in Refs. 34 and 35. The low-energy spectrum of the $2$-channel Kondo model with $J_a = J_b$ shows $SO(5)$ rotational symmetry, in the sense that the degeneracy factors of the eigenstates are subject to dimensions of its irreducible representations.

Returning back to the present Hamiltonian, it is confirmed that the spectra of low-energy eigenvalues on the unstable fixed points are identical to those obtained for the $2$-channel Kondo model with $J_a = J_b$, see Table III. Therefore, we describe these unstable fixed points as the $2$-channel Kondo ($2$-chK) ones.

### 4.2 Phase diagram of the generalized Anderson model for a vibrating magnetic ion

From the energy spectra obtained by the NRG calculations, we determine the ground-state phase diagram which is shown in Fig. 4. The parameter space is divided into two distinct areas. The left part is characterized by the $s$-type energy spectrum and the right part by the $p$-type one. On the boundary, the energy spectrum is of the $2$-chK type. On the line of $U = 0$, the $s$-type energy spectrum always appears. Therefore the line of $2$-chK fixed points does not merge together to the $U = 0$ line but approaches it asymptotically.

The NRG calculations reveal that physical properties of the system at finite temperatures are sometimes quite different even if two different sets of parameters belong to the region of the same fixed point at zero temperature. Therefore, in addition to the analysis of the low temperature energy spectra, we have to investigate finite temperature behaviors of physical quantities at each point of the parameter space.

First, we focus on the left side of the $2$-chK line. On the boundary, the energy spectrum is of the $2$-chK type. The left region is characterized by the $s$-type energy spectra and the right one by the $p$-type.

### Table I

| NRG step $n$ | even | odd |
|-------------|------|-----|
| $s$-type fixed point | $[2n + 2, 0, 0]$ | $[2n + 2, 0, 0]$ |
|           | $[2n + 3, ± \frac{1}{2}, 0]$ | $[2n + 3, ± \frac{1}{2}, 0]$ |
|           | $[2n + 4, 0, 0]$ | $[2n + 4, 0, 0]$ |
| $p$-type fixed point | $[2n + 2, 0, 1]$ | $[2n + 2, 0, 1]$ |
|           | $[2n + 3, ± \frac{1}{2}, 0]$ | $[2n + 3, ± \frac{1}{2}, 0]$ |
|           | $[2n + 4, 0, 1]$ | $[2n + 4, 0, 1]$ |

Table I. Sets of $[J_1, J_2, J_3, J_4, J_5, J_6, J_7, J_8]$ of the ground states at the $n$-th NRG step depending on the types of the fixed points.

### Table II

| $s$-type fixed point | $[1, 0, 0]$ | $[1, 0, 1]$ |
|----------------------|------------|------------|
| 0th                  | 0          | 0.800048   | 2          |
| 1st                  | 1.600095   | 3.400143   | 2          |
| 2nd                  | 1.695754   | 2.495802   | 6          |
| 3rd                  | 3.200191   | 2.997488   | 2          |

Table II. The low energy spectra of the $s$-type fixed point at an even number of the NRG steps for the sets of the quantum numbers, $[1, 0, 0]$ and $[1, 0, 1]$. In this table, $N_{\text{tot}}$ is counted from the total number of sites. The energy eigenvalues and their degeneracy factors are tabulated up to the third excited states. The low energy spectra of the $p$-type fixed points can be obtained by the inversion of the total parity $P$.

### Table III

| $s$-chK | $p$-chK |
|---------|---------|
| $Q, S^\text{tot}_{ch}$ | $Q, S^\text{tot}_{ch}$ |
| $SO(5)$ | $E_{\text{NRG}}$ |
| $[0, \frac{1}{2}, 1]$ | $(0, \frac{1}{2}, 0)$ | 1 | 0 |
| $[±1, 0, 0]$ | $(±1, 0, \frac{1}{2})$ | 4 | 0.125 |
| $[±1, 0, 1]$ | $(±1, 0, \frac{1}{2})$ | 4 | 0.125 |
| $[0, \frac{1}{2}, 0]$ | $(0, \frac{1}{2}, 0)$ | 5 | 0.505 |
| $[0, \frac{1}{2}, 1]$ | $(0, \frac{1}{2}, 1)$ | 4 | 0.637 |
| $[±1, 0, 0]$ | $(±1, 1, \frac{1}{2})$ | 4 | 0.637 |
| $[±1, 0, 1]$ | $(±1, 1, \frac{1}{2})$ | 1 | 1.013 |

Table III. Correspondence relation of the low energy eigenstates of the $2$-chK fixed point between the present model and the $2$-channel Kondo model at an even number of the NRG steps. In this table, $Q$ is defined by the difference between $N_{\text{tot}}$ and the total number of sites. Spin degeneracy is not counted in this table. The right part of the table is from Table II in Ref. 35 with spin $S$ and channel spin $S_{ch}$ for the $2$-channel Kondo model. *There are doubly degenerate states.

**Fig. 4.** (Color online) The phase diagram in the parameter space of $V_1$ and $U$ for $V_0 = \omega = 0.2$. On the boundary, the energy spectrum is of the $2$-chK type. The left region is characterized by the $s$-type energy spectra and the right one by the $p$-type. In the region between the green and blue dashed lines, the plateau of $S_{\text{imp}}$ at $k_B \log 2$ disappears.

2-chK type. On the line of $U = 0$, the $s$-type energy spectrum always appears. Therefore the line of $2$-chK fixed points does not merge together to the $U = 0$ line but approaches it asymptotically.

The NRG calculations reveal that physical properties of the system at finite temperatures are sometimes quite different even if two different sets of parameters belong to the region of the same fixed point at zero temperature. Therefore, in addition to the analysis of the low temperature energy spectra, we have to investigate finite temperature behaviors of physical quantities at each point of the parameter space.

First, we focus on the left side of the $2$-chK line. On the line of $U = 0$ this model is equivalent to the spin-
ful YA model. In the weak electron-phonon coupling regime main source of kinetic energy comes from the hybridization with the $s$-wave conduction electrons and the phonon-assisted hybridization with the $p$-wave channel is a weak perturbation. In this paper we characterize this regime by the renormalized Fermi chain (RFC). When $V_1$ increases, the PD is formed and the degeneracy is lifted at low temperatures by the Yu and Anderson type Kondo effect, expressed as $s$-YAK in Fig. 4. Now, we gradually increase Coulomb interaction $U$, starting from the parameter region where temperature dependence of physical quantities is of the RFC type. The impurity begins to behave as a localized spin and then the spin is screened mainly by the $s$-wave conduction electrons. This regime is called $s$-channel Kondo ($s$-chK) in Fig. 4. In the parameter region between RFC and $s$-chK, the essence of the physics can be understood based on the local Fermi liquid theory.$^{36,37}$

Next, we discuss the right part of the phase diagram. Concerning the strong $U$ regime, it is easy to understand that the local moment is screened mainly by the $p$-wave conduction electrons, which is called $p$-channel Kondo ($p$-chK). When $U$ is not important compared with $V_1$, the picture of the PD is valid, while the temperature dependence of physical quantities is different from that in the $s$-YAK parameter region in addition to the difference in the energy spectra. We denote this region as $p$-YAK in Fig. 4. In the following subsections, we will discuss details of physical properties for various parameters, including the difference between the $s$-YAK and $p$-YAK.

### 4.3 Three-site problem

At this point, it is instructive to consider the three-site problem, which consists of $f$, $s_0$ and $p_0$ sites. The

![Fig. 5. (Color online) The line of level crossing in the parameter space of $V_1$ and $U$ obtained from the three-site two-electron problem for $V_0 = \omega = 0.2$. The color grade corresponds to the magnitude of $\log|E_e - E_o|$, where $E_e$ and $E_o$ are the ground state energies with even and odd parity, respectively. In the left part of the deep blue line, $E_e$ is lower than $E_o$.](image)

![Fig. 6. (Color online) $U$ dependence of the difference between $E_e$ and $E_o$ for the three-site problem with two electrons: $V_0 = \omega = 0.2$ and $V_1 = 0.174$.](image)

![Fig. 7. (Color online) (a) $U$ dependence of $|\Psi_{e-e}|^2$ and $|\Psi_{o-e}|^2$ obtained for the three-site two-electron problem with $V_0 = \omega = 0.2$ and $V_1 = 0.174$. (b) $U$ dependence of $\langle q^2 \rangle_e$ and $\langle q^2 \rangle_o$, which are the expectation values of the square of the ion displacement calculated from $\Psi_{even}$ and $\Psi_{odd}$.](image)
Hamiltonian is given by

\[ H_{\text{site}} = V_0 \sum_{\sigma} \left\{ s_{\sigma}^+ f_{\sigma} + \text{h.c.} \right\} + V_1 \sum_{\sigma} \left\{ p_{\sigma}^+ f_{\sigma} + \text{h.c.} \right\} (a + a^\dagger) + \hbar \omega a^+ a + \frac{U}{2} \left( \sum_{\sigma} f_{\sigma}^+ f_{\sigma} - 1 \right)^2, \]

where the site suffix "0" is suppressed. It is easy to obtain the exact eigenvalues and eigenstates by using the exact diagonalization method. In the following examples the number of phonon excitations is kept up to 50 and \( V_0 \) and \( \omega \) are fixed to 0.2.

Figure 5 shows the magnitude of \( \log |E_e - E_o| \) in the two-dimensional parameter space of \( V_1 \) and \( U \), where \( E_e \) (\( E_o \)) is the ground state energies with even and odd parity. In the figure there is a line of level crossing between \( E_e \) and \( E_o \). In the left (right) part of the line, \( E_e \) (\( E_o \)) is lower than \( E_o \) (\( E_e \)). Figure 6 shows \( U \) dependence of the difference between \( E_e \) and \( E_o \) with \( V_1 \) fixed to 0.174. Clearly there is similarity between Fig. 4 and Fig. 5.

From the view point of parity, every component of wave functions is classified into four groups, \( \Psi_{e-e}, \Psi_{e-o}, \Psi_{o-e}, \) and \( \Psi_{o-o} \). For example, means a linear combination of the components whose electron parts have even parity and phonon parts odd parity. Clearly an eigenstate with even total parity is written as

\[ \Psi_{\text{even}} = \Psi_{e-e} + \Psi_{e-o}, \]

while one with odd total parity as

\[ \Psi_{\text{odd}} = \Psi_{o-e} + \Psi_{o-o}. \]

Concerning the three-site two-electron problem, the bases for a given parity are listed in Table IV.

![Table IV](image)

The wave functions are dominated by components with even phonon numbers. This fact is clearly seen in Fig. 7(a). Therefore the total parity is predominantly determined by the nature of singlet formation, even parity for the \( f - s \) singlet while odd parity for the \( f - p \) singlet. The upper critical \( U \) shown in Fig. 6 corresponds to the point where the two screening mechanisms compete in the same way as the 2-chK fixed point shown in the phase diagram for the bulk system, Fig. 4.

The line of level crossing shown in Fig. 5 is qualitatively similar to the phase boundary obtained by the NRG calculations, Fig. 4. We would like to point out that the three-site Hamiltonian corresponds to the initial step of the NRG procedure and the ground state of the two-electron problem has the different parity depending on the nature of the singlet bond as discussed in §4.1, see also Table I.

### 4.4 Strong correlation regime \((U \gg \omega \gg T)\)

Firstly, we discuss physical properties in the strong \( U \) regime where the relation, \( U \gg \omega \gg T \), holds. In this regime multi phonon excitation processes are not important. Because of the strong \( U \), the localized orbital behaves as a local moment which is coupled with the s-wave and p-wave conduction electrons. With lowering temperature, the local moment is screened by the conduction electrons and the main screening channel changes depending on relative strength between \( V_0 \) and \( V_1 \). In the same way as the conventional impurity Anderson model is mapped to the spin 1/2 Kondo model,\(^{38}\) we consider the projected Hilbert space where the vacuum and doubly occupied states of the impurity orbital are prohibited. We treat both of the conventional hybridization term \( V_0 \) and the phonon-assisted one \( V_1 \) in the Hamiltonian (2.9) as perturbation terms. After some calculations, a generalized Kondo model is obtained as

\[ H_{\text{Kondo}} = \sum_{\sigma \alpha} \sum_{k} \sum_{\ell = 0,1} \varepsilon(k) c_{\alpha \sigma}^\dagger(k) c_{\alpha \sigma}(k) + \hbar \omega a^\dagger a + H_{\text{H}}, \]

\[ H_{\text{H}} = - \sum_{kk'} \sum_{\alpha \beta} \sum_{\ell = 0,1} \left\{ J_{0,0} c_{\alpha \sigma}^\dagger(k) [\sigma]_{\alpha \beta} c_{\beta \sigma}(k') \cdot S + J_{1,0} q c_{\alpha \sigma}^\dagger(k) [\sigma]_{\alpha \beta} \cdot S + \text{h.c.} \right\} + J_{1,1} q^2 c_{\alpha \sigma}^\dagger(k) [\sigma]_{\alpha \beta} c_{\beta \sigma}(k') \cdot S, \]
where \( S = f_0^2 \langle \sigma \rangle_{\alpha\beta} f_\beta \) with \( \sigma \) being the vector of Pauli matrices and \( q = (a + a^\dagger) / \sqrt{2} \). The coupling constants \( J_{0,0}, J_{1,0} \) and \( J_{1,1} \) are written as
\[
\begin{align*}
J_{0,0} &\equiv V_0^2 \left\{ \frac{1}{\epsilon_f} - \frac{1}{\epsilon_f + U} \right\}, \\
J_{1,0} &\equiv V_0 \sqrt{2} V_1 \left\{ \frac{1}{\epsilon_f} - \frac{1}{\epsilon_f + U} \right\}, \\
J_{1,1} &\equiv 2V_1^2 \left\{ \frac{1}{\epsilon_f} - \frac{1}{\epsilon_f + U} \right\}.
\end{align*}
\]

The term proportional to \( J_{1,0} \) corresponds to scattering processes from the s-wave conduction electrons to the p-wave ones and vice versa. Similarly, the term proportional to \( J_{1,1} \) describes scattering processes within the p-wave conduction electrons. In the strong correlation regime, effects of electron-phonon coupling are suppressed by Coulomb interaction. Therefore we may regard the effects of phonon emission or absorption processes as a renormalization of the coupling constant by taking average over the phonon degree of freedom,
\[
H_{\text{div}} \approx - \sum_{kk'} \sum_{\alpha\beta} \left\{ J_{0,0} c_{\alpha\kappa}^\dagger(k) [\sigma]_{\alpha\beta} c_{\beta}(k') \cdot S \right\} + J_{1,1} q^2 c_{1\alpha}(k) [\sigma]_{\alpha\beta} c_{1\beta}(k') \cdot S \right\},
\]
where \( \langle q \rangle \), the thermal averages of \( q \), vanishes. Even if the electron-phonon coupling is weak, \( \langle q^2 \rangle \) is not zero due to the zero point fluctuations.

In Figs. 8 and 9 we use a set of parameters, \( V_0 = \omega = 0.2 \) with the symmetric condition \( U = -2\epsilon_f = 2.0 \). When \( V_1 \) is relatively small, \( T \chi_s \) increases close to 0.25 which corresponds to the local moment limit. With increasing \( V_1 \), phonon-assisted hybridization suppresses the enhancement of \( T \chi_s \).
4.5 Non-interacting case \((U = 0)\)

For discussions on the non-interacting case we fix the set of parameters \(V_0 = V_1 = 0.2\) and \(U = 0\). In this subsection we use frequency of phonon \(\omega\) as a parameter to change the strength of electron-phonon coupling, which is an alternative to control \(V_1\) with a fixed \(\omega\).

Entropy of the impurity site \(S_{\text{imp}}\) is shown in Fig. 10(a) for various \(\omega\). As \(\omega\) decreases, the plateau of entropy at \(k_B\log 2\) develops owing to the formation of the PD. Figure 10(b) summarizes results on the entropy in \(\omega - T\) plane. Typical YAK behaviors are observed in the parameter range from \(\omega = 0.238\) to 0.280. The middle of the blank area between the blue triangle and green circle regions corresponds to the Kondo temperature for the YAK effect.

In Fig. 11 the spin (charge) susceptibility of the impurity, \(T\chi_s = 0.25 T\chi_c\), is shown for various \(\omega\). When \(\omega\) is lowered, \(T\chi_s = 0.25 T\chi_c\) is suppressed since strong electron-phonon coupling increases the binding energy of the PD.

\[
\langle q^2 \rangle \approx 0.5
\]

The estimated value close to 1 seems to be reasonable.

\[
\frac{J_{1,1} \langle q^2 \rangle}{J_{0,0}} \approx 1.12.
\]
4.6 Effect of finite $U$ in the weak electron-phonon coupling regime

Next we choose the set of parameters $V_0 = 2V_1 = \omega = 0.2$, where screening by the $s$-wave conduction electrons dominates over the $p$-wave ones. To investigate the effects of Coulomb interaction, we show temperature dependence of the physical quantities, the entropy of the impurity ion $S_{\text{imp}}$ in Fig. 13, the spin susceptibility $T\chi_s$ in Fig. 14(a) and the charge susceptibility $T\chi_c$ in Fig. 14(b). When $U$ is small, $S_{\text{imp}}$ monotonically decays to zero. $T\chi_s$ and $T\chi_c$ also go to zero without any plateau. Therefore, we conclude that the physical properties correspond to the RFC regime in Fig. 4. When $U$ increases, the impurity orbital begins to behave as a local moment. Actually, the plateau region in Fig. 13 is broadened with increasing $U$. Correspondingly, $T\chi_s$ is enhanced and shows a maximum close to 0.25 while $T\chi_c$ is suppressed, which are signatures of a local moment. As already mentioned, the energy spectra are characterized by the $s$-type fixed point for any $U$. However the physical properties cross over from the RFC behaviors to the $s$-chK ones with increasing $U$.

4.7 Effect of finite $U$ in the strong electron-phonon coupling regime

In this subsection we show results of NRG calculations for a strong electron-phonon coupling case, $V_0 = V_1 = \omega = 0.2$. We will show, in Figs. 15(a) and 16 we see two distinct temperature dependence of $S_{\text{imp}}$ in the course of release of entropy from the plateau at $k_B \log 2$.

For $U < 1.4$ shown in Fig. 15(a), the electron-phonon coupling is relatively more important than the Coulomb interaction. In this region, the Coulomb interaction can be treated as a perturbation to the PD. For the non-interacting case the plateau of entropy at $k_B \log 2$ is not suppressed even at low temperatures. Because of the strong electron-phonon coupling we expect that the YAK temperature is much lower than $10^{-10}$. For $U > 0$, the low temperature energy spectrum is of the $p$-type. In §3.2, we showed that the Coulomb in-
interaction lifts the degeneracy of the PD in a similar way as a transversal magnetic field lifts degeneracy of a free spin. When $U$ is smaller than 1.4, it is expected that low-energy physics of the impurity is identified as Yu and Anderson type Kondo effect under the "transverse field", which is characterized by $p$-YAK in the phase diagram, Fig. 4. Therefore, it is useful for us to compare the present results with those of conventional spin 1/2 Kondo model under magnetic field. It is shown for the latter model that when the magnetic field is larger than Kondo temperature behavior of heat capacity approaches to a Schottky form (see Fig. 15 in Ref. 39). The lower panel of Fig. 15 shows $S_{\text{imp}}$ at $U = 0.01$ fitted by the Schottky form with $\Delta = 3.9 \times 10^{-5}$. Let us compare this $\Delta$ with the energy gap between the PD, namely $\Delta_{\text{PD}}$. To estimate $\Delta_{\text{PD}}$ it is appropriate to use a renormalized coupling constant $\lambda'$ instead of the bare $\lambda(\equiv -V_1/\omega)$.

We can estimate $\lambda'$ from the NRG calculations by using the relation $\langle q^2 \rangle = (16\lambda'^2 + 1)/2$. In this way $\Delta_{\text{PD}}$ is estimated to be $2.62 \times 10^{-5}$ for $U = 0.01$ by using $\langle q^2 \rangle = 5.75$. It is important to note that there is a notable deviation at low temperatures from the Schottky form. It indicates that energy spectrum at low temperatures is not gapped but continuous, which is consistent with the fact that even with a finite $U(\neq 0)$ the low temperature properties are described by a local Fermi liquid coupled with the $p$-wave conduction electrons.

We comment on the transition from the $s$-YAK regime to the $p$-YAK regime in the case of strong electron-phonon coupling. Let us start from the noninteracting case, $U = 0$. As we have discussed in §4.5 Kondo temperature of the YAK effect $T_{\text{YAK}}$ is generally small and becomes extremely small as the binding energy $|E_{\text{PD}}|$ gets larger, see Fig. 10(b). The Kondo energy, $k_B T_{\text{YAK}}$, is nothing but the energy gain at the $s$-type fixed points. On the other hand, the Coulomb interaction is favorable to the $p$-type fixed points and $\Delta_{\text{PD}}$ is its energy gain. Therefore, the transition takes place when $k_B T_{\text{YAK}} \sim \Delta_{\text{PD}}$. Since $k_B T_{\text{YAK}}$ is extremely small for strong electron-phonon coupling, the transition takes place close vicinity of the $U = 0$ line.

For $U \geq 1.5$ electrons in the impurity orbital behave as a local moment and it is quenched dominantly by the $p$-wave conduction electrons. Actually, in Fig. 16 there are plateaus of entropy at $k_B \log 2$ and the entropy is released in the same temperature dependence as the usual Kondo effect.

Lastly, let us discuss the intermediate parameter region, see Fig. 4. In the region between green and blue dashed lines, the entropy decays to zero without any plateau. It seems that the Coulomb interaction and the electron-phonon coupling are competing and almost balanced each other, leading to almost monotonic temper-
4.8 The line of 2-channel Kondo fixed points

Finally we discuss physical properties on the line of 2-chK fixed points shown in Fig. 4. On the line, energy spectra at low temperatures are always characterized by the 2-chK type. For the strong Coulomb interaction regime, energy spectra are always characterized by the 2-chK fixed points shown in Fig. 4. On the other hand, the magnitude of the local moment $\langle S_f^2 \rangle$ increases from 0.375 to 0.75. The former number corresponds to the free orbital limit, while the latter to the local moment limit. The curve of $\langle S_f^2 \rangle$ is concave-downward. These results support the view that the degree of freedom to be screened by conduction electrons smoothly transfers from the ion displacement to the spin degrees of freedom of local moment with increasing $U$.

5. Conclusion and future problems

In this paper we have discussed Kondo effects when a magnetic ion is vibrating in a harmonic potential. The central issue is the competition between the Coulomb and electron-phonon interactions. To treat the problem, a generalized impurity Anderson model is derived by taking account of vibrational mode of oscillations. Associated with phonon absorption or emission, a new channel opens for hybridization of the localized orbital with conduction electrons. Suppose the localized orbital is described by an $\ell$-spherical wave, then the new channels are hybridization with the $\ell \pm 1$ partial waves. In the simplest case of the $s$-wave symmetry of the localized orbital, the new channel is the mixing with the $p$-partial waves.

To proceed further, we have restricted the ion oscillation to one dimension, in which case only one component screened by the conduction electrons are not the spin degrees of freedom of the impurity orbital but the ion displacements of the PD.

To observe the crossover behavior, we show thermal average of square of the ion displacement $\langle q^2 \rangle$ and magnitude of the local moment $\langle S_f^2 \rangle$ calculated at low temperatures. Figure 18 shows $\langle q^2 \rangle$ and $\langle S_f^2 \rangle$ calculated for the sets of parameters on the line of 2-chK fixed points in Fig. 4. When $U$ increases along the line, $\langle q^2 \rangle$ is suppressed by Coulomb interaction and approaches to 0.5 which corresponds to the zero point fluctuations. $\langle q^2 \rangle$ decreases monotonically, showing a concave curve as a function of $U$. On the other hand, the magnitude of the local moment $\langle S_f^2 \rangle$ increases from 0.375 to 0.75. The former number corresponds to the free orbital limit, while the latter to the local moment limit. The curve of $\langle S_f^2 \rangle$ is concave-downward. These results support the view that the degree of freedom to be screened by conduction electrons smoothly transfers from the ion displacement to the spin degrees of freedom of local moment with increasing $U$.

Fig. 17. (Color online) Temperature dependence of $T\chi_s$ (a) and $T\chi_c$ (b) in the strong electron-phonon coupling regime, $V_0 = V_1 = \omega = 0.2$. For the $U = 0$, the relation $T\chi_s = 0.25T\chi_c$ is valid. Unlike the weak electron-phonon coupling case, the enhancement of $T\chi_s$ by Coulomb interaction is weak for $U < 2.0$. $T\chi_s$ starts to show a maximum for $U > 2.0$ and becomes close to 0.25 as $U$ is increased.

Fig. 18. (Color online) $U$ versus $\langle q^2 \rangle$ and $\langle S_f^2 \rangle$ with $V_0 = \omega = 0.2$. The sets of the parameters, $V_1$ and $U$, are chosen to correspond to each points on the red line with squares in Fig.4.
among the three $p$-partial waves is relevant. With this reduction, the rotational symmetry of the original system is lowered to the inversion symmetry. This model still shows rich variety of interesting physics which includes different limiting cases: conventional $s$-wave Kondo effect, phonon-assisted $p$-wave Kondo effect and Yu-Anderson type Kondo effect.

The model has been analyzed by using the NRG scheme and it has been shown that the low-energy fixed points belong to one of the two different classes which are characterized by the $s$-type or $p$-type fixed points. On the boundary we find generically the 2-chK fixed points. Surprisingly, not only the $s$-chK but also the YAK regions are continuously connected to the local Fermi liquid. It is also a new finding that the YAK effect which has been discussed for a system with strong electron-phonon coupling but without any effect of electron-electron correlation is actually very sensitive to the Coulomb interaction.

With introduction of small $U$, the fixed point of the YAK effect changes from the $s$-type to the $p$-type.

Concerning the Kondo effects of a magnetic ion vibrating in the sea of conduction electrons, there are a number of interesting questions to be addressed in future. Response to magnetic fields may be different depending on where the system is located in the phase diagram. Especially, effect of magnetic field for the YAK effect would be very interesting in the region around the boundary of the 2-chK. For the present model interesting phase transitions take place close to the region of intermediate electron-phonon coupling, $V_0 \sim V_1$ and $V_1 \sim \omega$. When we consider a strongly anharmonic potential like a double well one, the condition for the occurrence of the YAK effect would be drastically modified. In view of the fact that there are some experimental indications that magnetic ions in some skutterudite compounds migrate among off-center positions, this might be an interesting question relevant to this class of materials.\textsuperscript{40-42}

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Appendix: Expansion of the overlap integrals within $O(Q)$

In this appendix we derive hybridization terms expanded within the first order of ion displacement by using the generalized gradient theorem.\textsuperscript{26} This theorem is applicable to the present model because the rotational symmetry $SO(3)$ is assumed in the total system including both the ion and the conduction electrons. First, let us transform the coordinate system from the conventional Cartesian form to the spherical tensor form. The position vectors of a conduction electron and the ion displacement $Q$ are transformed to

$$r_{1,\pm 1} = \pm \frac{1}{\sqrt{2}} (r_x \mp i r_y), \quad r_{1,0} = r_z,$$

$$Q_{1,\pm 1} = \pm \frac{1}{\sqrt{2}} (Q_x \pm iQ_y), \quad Q_{1,0} = Q_z.$$

One can show that the set of differential operators $\{\nabla_{1,m}\}$ defined by $\{r_{1,m}\}$ are first rank spherical tensor operators. Within $O(Q)$ the overlap integral is written as

$$V_{(k;\ell,m)}(Q)$$

$$= \frac{g}{\sqrt{\Omega}} \int d^3 r e^{-ik\cdot r} \psi_{\ell m}(r-Q)$$

$$\simeq \frac{g}{\sqrt{\Omega}} \int d^3 r e^{-ik\cdot r} \{ \psi_{\ell m}(r) - Q \cdot \nabla \psi_{\ell m}(r) \}.$$ 

$Q \cdot \nabla$ is expressed in the spherical tensor form by $\sum_m Q_{1,m} \nabla_{1,m}$ because of the $SO(3)$ symmetry. The spherical tensors can be expressed in terms of the spherical harmonics $|\ell, m\rangle$ and the Clebsch-Gordan coefficients $\langle \ell', m' | \ell, m \rangle$ by

$$\langle \ell', m' | \nabla_{1,m} | \ell, m \rangle$$

$$= \sqrt{\frac{\ell + 1}{2\ell + 3}} \langle \ell, m; m_1 | \ell', m' \rangle \left\{ \frac{\partial}{\partial r} - \frac{\ell}{r} \right\}$$

$$\times \delta_{\ell', \ell+1} \delta_{m', m+1}$$

$$- \sqrt{\frac{\ell}{2\ell - 1}} \langle \ell, m; m_1 | \ell', m' \rangle \left\{ \frac{\partial}{\partial r} + \frac{\ell + 1}{r} \right\}$$

$$\times \delta_{\ell', \ell-1} \delta_{m', m+1}. \quad (A.1)$$

After rewriting $e^{-ik\cdot r}$ by using the spherical wave expansion, the integrals expanded within the first order of $Q$ are given by

$$V_{(k;\ell,m)}(Q)$$

$$= i^{\ell} R_{\ell}(k) \sqrt{4\pi} Y_{\ell m}(\hat{k}) + \sum_{m_1=-1}^{1} Q^*_{1,m_1}$$

$$\times \left\{ \Gamma^+_{(\ell,m_1;m_1)} i^{-(\ell+1)} r_{\ell+1}(k) \sqrt{4\pi} Y_{\ell+1,m+m_1}(\hat{k}) \right.\right.$$

$$\left. + \Gamma^-_{(\ell,m_1;m_1)} i^{-(\ell-1)} r_{\ell-1}(k) \sqrt{4\pi} Y_{\ell-1,m+m_1}(\hat{k}) \right\}. \quad (A.2)$$

where $\Gamma^+(-)_{(\ell,m_1;m_1)}$ are defined by

$$\Gamma^+_{(\ell,m_1;m_1)} = \sqrt{\frac{\ell + 1}{2\ell + 3}} \langle \ell, m; m_1 | \ell + 1, m + m_1 \rangle. \quad (A.3)$$

$$\Gamma^-_{(\ell,m_1;m_1)} = \sqrt{\frac{\ell}{2\ell - 1}} \langle \ell, m; m_1 | \ell - 1, m + m_1 \rangle. \quad (A.4)$$

The radial integrals are represented by the spherical Bessel functions and the radial parts of $\psi_{\ell m}(r)$ as

$$R_{\ell}(k) \equiv \sqrt{\frac{4\pi}{2\ell + 1}} g \int dr r^2 j_{\ell}(kr) u_{\ell}(r),$$

$$r_{\ell+1}(k)$$
\[ \equiv \frac{4\pi}{V} g \int dr r^2 j_{r+1}(kr) \left\{ \frac{\ell}{r} - \frac{\partial}{\partial r} \right\} u_\ell(r), \quad (A.6) \]

\[ r_{\ell-1}(k) \equiv \frac{4\pi}{V} g \int dr r^2 j_{\ell-1}(kr) \left\{ \frac{\partial}{\partial r} + \frac{\ell + 1}{r} \right\} u_\ell(r). \quad (A.7) \]

Lastly we neglect the \( k \) dependence of the radial integrals and use the values at the Fermi momentum \( k_F \). After introducing the dimensionless ion displacement \( q(\equiv \alpha Q) \), we obtain eq. (2.7), where \( V_\ell \) and \( V^{(m;m')}_{\ell \pm 1} \) are defined by

\[ V_\ell \equiv i^{-\ell} R_\ell(k_F), \quad (A.8) \]

\[ V^{(m;m')}_{\ell \pm 1} \equiv i^{-(\ell \pm 1)} r_{\ell \pm 1}(k_F) R^{\pm}_{(m;m')} \quad (A.9) \]

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