Hubbard chains network on corner-sharing tetrahedra: Origin of the heavy-fermion state in LiV_2O_4

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We investigate the Hubbard chains network model defined on corner-sharing tetrahedra (the pyrochlore lattice) which is a possible microscopic model for the heavy-fermion state of LiV_2O_4. Based upon this model, we can explain transport, magnetic, and thermodynamic properties of LiV_2O_4. We calculate the spin susceptibility, and the specific-heat coefficient, exploiting the Bethe ansatz exact solution of the one-dimensional Hubbard model and Bosonization method. The results are quite consistent with experimental observations. We obtain the large specific-heat coefficient $\gamma \sim 222$ mJ/mol K^2.

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I. INTRODUCTION

Recently, it is discovered that a heavy-fermion (HF) state is realized in LiV_2O_4, a transition-metal oxide with a cubic spinel structure.[1–6] It has the largest specific-heat coefficient among *d*-electron systems, $\gamma \sim 420$ mJ/mol K^2.[1] The origin of the HF behavior without almost localized *f* electrons is still an important open issue. *Ab initio* band calculations suggest that geometrical frustration of the spinel structure in which *V* sites form a corner-sharing tetrahedra network (so-called pyrochlore lattice) may be important.[7–9] Actually, it is known that some geometrically frustrated electron systems in the vicinity of the Mott transition shows a HF behavior.[10–12] However, since the electron density of LiV_2O_4 is quarter filling, the above idea may not be directly applicable to this system. Nevertheless, it is expected that the geometrical frustration plays some crucial role. On the other hand, Anisimov *et al.* proposed that the t_{2g} band of *V* sites is splitted into localized and conduction parts by trigonal crystal field, and thus the system is simulated by the Kondo lattice model.[13]

Here, we would like to propose another microscopic model for the HF state from a quite different point of view. We pay attention to the fact that, as was shown by band calculations, electrons near the Fermi surface consist mainly of the t_{2g} orbitals of *V* ion which is quarter filled, and that the hybridization with *p* electrons of oxygen is small.[7,8] We will neglect trigonal field splitting, since it is smaller than the bandwidth by $\sim 1/10$.[7] Then we can see that each t_{2g} orbital on the corners of the pyrochlore lattice forms one-dimensional (1D)-like bands along each edge of tetrahedra (see Fig. 1). It is expected that the hybridization between these 1D bands is much suppressed by the geometrical configuration. In other words, we can say that to reduce the geometrical frustration the electronic structure maintains the 1D-like character. Actually, the band structure obtained from this consideration resembles qualitatively that of *ab initio* calculations.[7,8] This proposal is also supported by the following experimental observations. (i) Recent neutron-scattering measurements show that there exists antiferromagnetic spin fluctuation with a staggered wave vector $Q \sim 0.84a^*$.[6] This Q vector is close to that of the quarter filled 1D Hubbard model [$Q_{1D}=2\pi/(4d_{V\text{-}V}) \sim 0.71a^*$, $d_{V\text{-}V}$ is the distance between the nearest-neighbor *V* sites; see Ref. 6]. (ii) As temperature is raised, the resistivity increases monotonically like $\sim T$ for $T > T^*$, and is not saturated in contrast to *f*-electron-based HF systems.[5] Here T^* is the characteristic temperature which is analogous to the Kondo temperature of *f*-electron-based HF systems. The behavior is easily understood, if we identify T^* with a dimensional crossover temperature. Namely, T^* is regarded as a crossover temperature from 1D to 3D. For $T > T^*$, the 1D-like electronic structure gives rise *T*-linear resistivity.[14] (iii) Moreover, the Hall coefficient measured by Urano *et al.* is much small for $T > T^*$.[5] Since there exist several Fermi surfaces in this system, it is rather difficult to calculate the Hall coefficient from a microscopic model. However, this experimental fact does not contradict with the interpretation that for $T > T^*$ the system has 1D-like character. We show schematically the temperature dependence of the Hall coefficient and the resistivity of our model in Fig. 2. It is noted that these properties are not changed qualitatively even if the sample is not a single crystal, as in the case of some experimental situations.

Based upon these considerations, we construct the network of quarter filled Hubbard chains in directions (1, ±1, 0), (1, 0, ±1), and (0, 1, ±1), which is defined on the corner-sharing tetrahedra. We assume that the chains are coupled weakly with each other at the corners of tetrahedra. Because of 1D-like structure, electron correlation effect is much enhanced, leading to the large specific-heat coefficient. In this paper, we demonstrate this scenario by microscopic calculation. We show that the temperature dependence of the spin susceptibility calculated from our model is consistent with

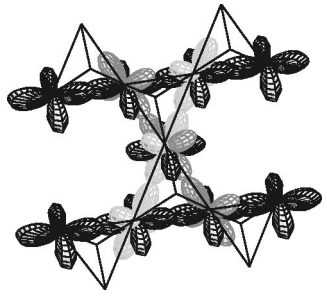

FIG. 1. Some portions of one-dimensional-like bands formed by the t_{2g} orbital on the pyrochlore lattice.

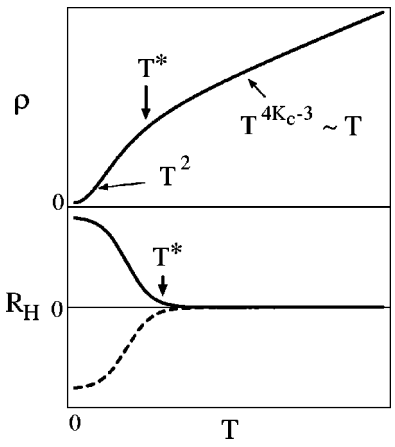

FIG. 2. A schematic view for the temperature dependence of the resistivity ρ and the Hall coefficient R_H of the Hubbard chains network model. In high-T regions, the Luttinger liquid parameter $K_c \sim 1$. The sign of R_H for $T<T^*$ depends on the curvature of the 3D Fermi surface formed in the low-energy scale.

experimental observations, and that the specific-heat coefficient is enhanced like $\gamma \sim 222$ mJ/mol K^2. A similar idea has been recently proposed by Fulde *et al.* who considered a network of 1D Heisenberg spin chains with spins 1 and 1/2.[15] However, since LiV_2O_4 is metallic, we believe that our model is more appropriate to discuss the HF state of this system.

II. HUBBARD CHAINS NETWORK MODEL

Based on the consideration presented in the Introduction, we construct the Hamiltonian of our model in the presence of a magnetic field $h(x_i)$,

$$H=\sum_{\alpha=1}^{6} H_{1\mathrm{D}}^{(\alpha)}+\sum_{\alpha\beta,\sigma,i} V_{\alpha\beta} c_{\alpha\sigma i}^{\dagger} c_{\beta\sigma i} - g\mu_{\mathrm{B}} \sum_{i} S_{\alpha i}^{z} h(x_i), \tag{1}$$

where $H_{1\mathrm{D}}^{(\alpha)}$ is the Hamiltonian of the 1D Hubbard model,

$$H_{1\mathrm{D}}^{(\alpha)}=-t\sum_{\sigma,i} c_{\alpha\sigma i}^{\dagger} c_{\alpha\sigma i+1}+\mathrm{H.c.}+U\sum_{i} n_{\alpha\uparrow i} n_{\alpha\downarrow i}. \tag{2}$$

$c_{\alpha\sigma i}$ ($c_{\alpha\sigma i}^{\dagger}$) is an annihilation (creation) operator for electrons on α chains, and $S_{\alpha i}^{z}=c_{\alpha\sigma i}^{\dagger}(\sigma_z/2)_{\sigma\sigma'} c_{\alpha\sigma' i}$. $H_{1\mathrm{D}}^{(1)}$, $H_{1\mathrm{D}}^{(2)}$, $H_{1\mathrm{D}}^{(3)}$, $\cdots H_{1\mathrm{D}}^{(6)}$ correspond to the chains in the (1, 1, 0), (0, 1, 1), (1, 0, 1), (0, 1, -1), (1, 0, -1), and (1, -1, 0) directions, respectively. Because of t_{2g} symmetry of d electrons, each chain cannot hybridize directly at the same points. However, in LiV_2O_4, it is possible that the hybridization between different chains realizes through p electrons of oxygen. Actually the hybridization between the chains should be nonlocal. This nonlocality makes the model quite complicated. Thus for simplicity, we assume that each Hubbard chains hybridizes at each corner of a tetrahedron. The hybridization parameter $V_{\alpha\beta}$ is given by

$$\hat{V}=V_{\alpha\beta}=\begin{pmatrix} 0 & V & V & V & V & 0 \\ V & 0 & V & 0 & V & V \\ V & V & 0 & V & 0 & V \\ V & 0 & V & 0 & V & V \\ V & V & 0 & V & 0 & V \\ 0 & V & V & V & V & 0 \end{pmatrix}. \tag{3}$$

Then the hybridization gives rise the doubling of 1D bands generating total 12 bands because of the geometrical structure of a tetrahedron. In spite of this simplification of the hybridization parameter, the band structure of this network model is roughly similar to that obtained by first-principles band calculations.[7,8] Thus we believe that our model captures the important features of LiV_2O_4. Comparing the band structure with that in Refs. 7 and 8, we choose $t=0.25$ eV. We use this parameter in the following calculations.

The issue of dimensional crossover from 1D to 3D has been studied extensively so far.[16–18] The basic idea of these previous works is to expand the free energy in terms of interchain couplings, and to apply Landau-Ginzburg type arguments. To avoid confusion, we would like to stress that our system is not an assembly of parallel chains as was considered in the previous studies, but a network composed of chains aligned in six different directions reflecting the topology of tetrahedra. However, we can apply the basic method of the dimensional crossover problem to our model. Following Boies *et al.*,[18] we use the Hubbard-Stratonovich transformation $V_{\alpha\beta} c_{\alpha\sigma i}^{\dagger} c_{\beta\sigma i} \rightarrow V_{\alpha\beta} c_{\alpha\sigma i}^{\dagger} \psi_{\beta\sigma}(x_i) + V_{\alpha\beta} \psi_{\alpha\sigma}^{\dagger}(x_i) c_{\beta\sigma i} + V_{\alpha\beta} \psi_{\alpha\sigma}^{\dagger}(x_i) \psi_{\beta\sigma}(x_i)$. Averaging over $c_{\alpha\sigma i}$ and $c_{\alpha\sigma i}$ with respect to the action of the 1D Hubbard model, we carry out the cumulant expansion in $V_{\alpha\beta}$ and h. Then, we have the partition function

$$Z=Z_{1\mathrm{D}} \int \mathcal{D}\psi \mathcal{D}\psi^{\dagger} e^{-S(\psi,\psi^{\dagger})}, \tag{4}$$

where $Z_{1\mathrm{D}}$ is the partition function of the 1D Hubbard model. The effective action is given by

$$S(\psi,\psi^{\dagger})=S^{(1)}+\sum_{n=2}^{\infty} S^{(n)}+\sum_{q} \langle S^z(q) S^z(-q)\rangle^{(1\mathrm{D})} h_q^2$$

$$+\sum V_{\alpha\beta_1} V_{\beta_2\alpha} \langle c_{\alpha\sigma_1 i_1} c_{\alpha\sigma_2 i_2}^{\dagger} S_{\alpha i_3}^{z}\rangle^{(1\mathrm{D})}$$

$$\times \psi_{\beta_1\sigma_1}^{\dagger}(x_1) \psi_{\beta_2\sigma_2}(x_2) h(x_3), \tag{5}$$

$$S^{(1)}=\int dx_1 dx_2 \psi_{\sigma}^{\dagger}(x_1)$$

$$\times [\hat{V}\delta(x_1-x_2)-\hat{V}^2 \hat{G}^{(1)}(x_1-x_2)] \psi_{\sigma}(x_2), \tag{6}$$

$$S^{(n)}=\frac{1}{n!}\sum G_{c\alpha}^{(2n)}(x_1,x_2,\ldots,x_{2n}) V_{\alpha\beta_1} V_{\beta_2\alpha} \cdots V_{\beta_{2n}\alpha}$$

$$\times \psi_{\beta_1\sigma_1}^{\dagger}(x_1) \cdots \psi_{\beta_{2n}\sigma_{2n}}(x_{2n}), \tag{7}$$

where $x_n=(\mathbf{x}_n, t_n)$, and $\langle \cdots \rangle^{(1\mathrm{D})}$ is a correlation function of the 1D Hubbard model. $\{\hat{G}^{(1)}(x)\}_{\alpha\beta}=G_{\alpha}^{(1)}(x)\delta_{\alpha\beta}$ with $G_{\alpha}^{(1)}(x)$ the single-particle Green's function of α chain, and

$G^{(2n)}_{c\alpha}(x_1,\ldots,x_{2n})$ is the connected $2n$-particle correlation function of α chain, $\langle c_1 c_2^\dagger \cdots c_{2n-1} c_{2n}^\dagger \rangle_c^{(1D)}$. $\hat{V}$ is a matrix with elements $V_{\alpha\beta}$.

In the presence of the hybridization V, the quasiparticle weight, which is the hallmark of the Fermi-liquid state, develops as the temperature is lowered.[18] To see this, it is sufficient to consider only up to $S^{(1)}$ term of Eq. (5). The pole of the single-particle Green's function $\hat{G}(k,\varepsilon)=\hat{G}^{(1)}(k,\varepsilon)[1-\hat{V}\hat{G}^{(1)}(k,\varepsilon)]^{-1}$ determines the quasiparticle energy spectrum $E_k \sim [2(1-\theta)v_c v_s/(v_c+v_s)]k \equiv v_F k$. Here v_c is the velocity of holon, and v_s is that of spinon. The quasiparticle weight is $z \sim 2\sqrt{v_c v_s}(\Delta k v_c/E_F)^\theta/(v_c+v_s)$, with $\Delta k = [4 V v_c^\theta (v_c v_s)^{-1/2} E_F^{-\theta}]^{1/(1-\theta)}$, $\theta=(K_c+1/K_c-2)/4$, K_c is the Luttinger liquid parameter of the charge sector, and E_F is the Fermi energy of the 1D Hubbard model. $S^{(n)}$ $(n \geqslant 2)$ terms are relevant perturbations to this Fermi-liquid state. As long as spontaneous symmetry breaking does not occur, the Fermi-liquid state is stable. At sufficiently high temperatures, we can treat $S^{(n)}$ $(n \geqslant 2)$ terms as small perturbations. In the following, we take into account only $S^{(2)}$ term. At low temperatures, effects of higher-order terms $S^{(n)}$ $(n \geqslant 3)$ are not negligible. To estimate the temperature range in which our approach is valid, we apply simple scaling argument to the action (5). The scaling equation for the effective coupling of $S^{(2)}$, which we denote g_4, is given by

$$\frac{dg_4}{d\ln\left(\frac{T_E}{T}\right)} = (1-K_c)g_4. \tag{8}$$

Then, g_4 grows to the order of unity at $T \sim (V/4t)^{4/(1-K_c)} T_F$, where $T_F \sim 4t$, the bandwidth of the 1D Hubbard model. Thus our approach is applicable for $T > T_0 \equiv (V/4t)^{4/(1-K_c)} T_F$. For $T < T_0$, our approximation will be less accurate quantitatively. As we will see later, T_0 is sufficiently small for the parameters we use.

Using the Bosonization rule and the operator product expansion for the U(1) Gaussian model and the level-1 SU(2) Wess-Zumino-Witten model, we can show that the leading term of $S^{(2)}$ is written as[19–21]

$$\begin{aligned} S^{(2)} \sim \frac{1}{2} \sum_{\alpha\beta_1\cdots\beta_4} \sum_{k,k',q} & V_{\alpha\beta_1} V_{\beta_2\alpha} \cdots V_{\beta_4\alpha} \\ & \times \Bigg(\frac{1}{4v_c^2} \langle \rho_\alpha(q)\rho_\alpha(-q)\rangle^{(1D)} \sum_{\sigma\sigma'} \psi^\dagger_{\beta_1\sigma}(k'+q) \\ & \times \psi_{\beta_2\sigma}(k') \psi^\dagger_{\beta_3\sigma'}(k-q) \psi_{\beta_4\sigma'}(k) + \frac{1}{2v_s^2} \\ & \times \langle S^+_\alpha(q) S^-_\alpha(-q)\rangle^{(1D)} \sum_{\sigma_1\sigma_2\sigma_3\sigma_4} \psi^\dagger_{\beta_1\sigma_1}(k'+q) \\ & \times \sigma_{\sigma_1\sigma_2} \psi_{\beta_2\sigma_2}(k') \psi^\dagger_{\beta_3\sigma_3}(k-q) \sigma_{\sigma_1\sigma_2} \psi_{\beta_4\sigma_4}(k) \Bigg). \end{aligned} \tag{9}$$

Here $\rho(q)=\Sigma_{\sigma,k} c^\dagger_{\sigma,k+q} c_{\sigma,k}$, $S^+_\alpha(q)=\Sigma_k c^\dagger_{\uparrow,k+q} c_{\downarrow,k}$, etc. In a similar manner, we can rewrite the last term of Eq. (5) as

$$\begin{aligned} & \frac{1}{v_s} \sum_{\alpha\beta_1\beta_2} V_{\alpha\beta_1} V_{\beta_2\alpha} \\ & \times \Bigg(\sum_{q\sim 0} \sum_\omega \chi^{1D}_u(q,\omega) \psi^\dagger_{\beta_1\sigma_1,k+q} \sigma^x_{\sigma_1\sigma_2} \\ & \times \psi_{\beta_2\sigma_2,k} h_q + \sum_{q\sim Q} \sum_\omega \chi^{1D}_s(q,\omega) \\ & \times \psi^\dagger_{\beta_1\sigma_1,k+q} \sigma^z_{\sigma_1\sigma_2} \psi_{\beta_2\sigma_2,k} h_q \Bigg). \end{aligned} \tag{10}$$

Here $\chi^{1D}_u(q\sim 0,\omega)$ and $\chi^{1D}_s(q\sim Q_0,\omega)$ are the uniform and staggered parts of the spin susceptibility, respectively, for the 1D Hubbard model. $Q_0=\pi/2$ in the quarter filling case.

III. MAGNETIC PROPERTIES

In this section we consider the magnetic properties of the system. Applying random-phase approximation, we compute the spin susceptibility,

$$\begin{aligned} \chi(q) &= -T\delta^2 \ln Z/\delta h_q^2 \\ &= \sum_{\alpha\beta} \{\hat{\chi}^{1D}(q)[1-\hat{\Gamma}(q)\hat{\chi}^{1D}(q)]^{-1}\}_{\alpha\beta}, \end{aligned} \tag{11}$$

where $\{\hat{\chi}^{1D}(q)\}_{\alpha\beta}=\chi^{1D}_\alpha(q_\alpha)\delta_{\alpha\beta}$ with $q_1=q_2=q_x+q_y$, $q_3=q_4=q_y+q_z$, $q_5=q_6=q_x+q_z$, $q_7=q_8=q_y-q_z$, $q_9=q_{10}=q_x-q_z$, and $q_{11}=q_{12}=q_x-q_y$. $\{\hat{\Gamma}(q)\}_{\alpha\beta}=1/v_s^2 \Sigma_k \tilde{G}^0_{\alpha\beta}(k+q)\tilde{G}^0_{\alpha\beta}(k)$, with $\tilde{G}^0_{\alpha\beta}=\{\hat{V}\hat{G}^0\hat{V}\}_{\alpha\beta}$, and $\hat{G}^0=[\hat{V}-\hat{V}^2\hat{G}^{(1)}]^{-1}$. It is noted that in the denominator of Eq. (11) the single-particle Green's function $\hat{G}^0$ appears. Equation (11) implies that as the quasiparticle weight develops, the spin-spin correlation between Hubbard chains which is mediated by two-particle hopping is enhanced. This point is important for the following arguments. Although we know the low-energy expression of $G^{(1)}(x,t)$, it is difficult to carry out the Fourier transform analytically.[22] For simplicity, we approximate the anomalous exponent of $G^{(1)}(x,t)$ as $\theta \approx 0$. Actually θ is sufficiently small for intermediate strength of U, e.g., $\theta=0.059$ $(K_c=0.618)$ for $U/4t=2$, and $\theta=0.03$ $(K_c=0.71)$ for $U/4t=1$. Then the Fourier transform of $G^{(1)}(x,t)$ is given by

$$\begin{aligned} G^{(1)R}_L(k,\varepsilon) = & \frac{-2iA\sqrt{v_c v_s}}{(2\pi)^2 T(v_c-v_s)} B\left(\frac{1}{4} - i\frac{v_s(\varepsilon-kv_c)}{2\pi(v_c-v_s)T}, \frac{1}{2}\right) \\ & \times B\left(\frac{1}{4} - i\frac{v_c(\varepsilon-kv_s)}{2\pi(v_c-v_s)T}, \frac{1}{2}\right), \end{aligned} \tag{12}$$

where $B(x,y)$ is the beta function, and A is a nonuniversal prefactor which depends on model parameters. Unfortunately we do not know the exact value of A. In the following, to avoid overestimating electron correlation effects, we use the noninteracting value of A. We now calculate the uniform

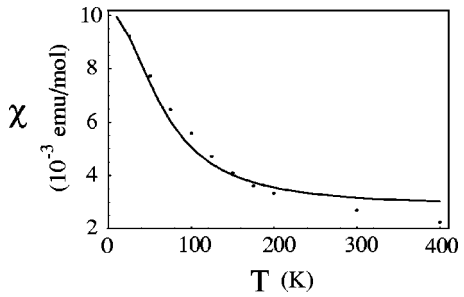

FIG. 3. Calculated result of temperature dependence of the spin susceptibility (solid line). The dots are experimental data quoted from Refs. 5 and 3.

susceptibility $\chi(q=0)$ from Eqs. (11) and (12). In the numerical calculation, we neglect the off-diagonal components of $\hat{G}^0$ and $\hat{\chi}$, which may give subdominant corrections. We choose the parameter $4t=1$ eV, and $U=2$ eV, the value suggested from photoemission measurements.[23] Using the Bethe ansatz exact solution, we can obtain v_c, v_s, and $\chi^{1D}(0)=1/(2\pi v_s)$.[24–26] We determine V by fitting the uniform spin susceptibility with experimental data. The result is shown in Fig. 3. We set $V/t=0.4506$. For this parameter, $T_0/T_F \sim 10^{-8}$. Thus we can apply our results to the wide temperature range including sufficiently low-temperature regions. The spin susceptibility consists of the Pauli paramagnetic term and the temperature-independent Van Vleck term. To fit to experimental data, we set the Van Vleck term $\chi_{VV} \sim 2.1\times 10^{-3}$ emu/mol. It is noted that the Curie-like temperature dependence is not due to the presence of local moment as in the case of dense Kondo systems, but caused by the development of 3D-like magnetic correlation between Hubbard chains. As temperature decreases, the single-particle weight becomes large, leading to the enhancement of 3D correlation mediated by two-particle hopping.

IV. SPECIFIC-HEAT COEFFICIENT: HEAVY-FERMION STATE

Let us consider the specific-heat coefficient which characterizes the HF behavior. According to Eq. (4), the free energy is given by the sum of the 1D part and the Fermi-liquid part. Thus the specific-heat coefficient is expressed as $\gamma=\gamma_{1D}+\gamma_{FL}$. It should be noted that this expression is valid only around the crossover temperature T^*, since in the sufficiently low-temperature region the higher-order terms of $S^{(n)}$ which are neglected in our approximation will cancel the 1D-like contribution, and the conventional Fermi-liquid result must be recovered. Thus $\gamma \sim \gamma_{FL}$ in the low-temperature region where the system is in the 3D Fermi-liquid state.

We calculate the Fermi-liquid part γ_{FL} taking into account contributions from spin fluctuations. Since in the 1D Hubbard model the staggered component of the spin fluctuation is dominant over the uniform one, the antiferromagnetic spin fluctuation gives leading corrections to the self-energy. This is consistent with recent neutron-scattering measurements.[6] The propagator for the antiferromagnetic spin fluctuation is obtained from Eq. (11). We calculate numerically the Fourier transform of the staggered spin susceptibility

$$\chi_s^{1D}(x,t)=e^{iQ_0x}\,\mathrm{Im}\,(1/\{2\pi^2[x^2-v_c^2(t-i\delta)^2]^{K_c/2} \times[x^2-v_s^2(t-i\delta)^2]^{1/2}\})\theta(t),$$

which is divergent for $q=Q_0$.[22] This divergence is cut off by the momentum scale at which the crossover from 1D to 3D system occurs, i.e., $q\sim\Delta k$. Since the nonuniversal prefactor of $\chi_s^{1D}(x,t)$ is unknown for finite U, we use the prefactor of noninteracting systems to simplify the calculation. $\chi_{11}(q,\omega)$ has peaks at $\mathbf{Q}=(Q_0,0,0)$, $(0,Q_0,0)$, and $(Q_0/2,Q_0/2,Q_0/2)$. Expanding Eq. (11) around one of these peaks, we have

$$\chi_{11}(\mathbf{Q}+\mathbf{q},\omega)\sim\frac{\chi_0(\mathbf{Q})}{1+\xi_x^2q_x^2+\xi_y^2q_y^2+\xi_z^2q_z^2-i\omega/\Gamma_q}. \quad (13)$$

Here $\chi_0(\mathbf{Q})=\{\hat{\chi}^{1D}(\mathbf{Q})[1-\hat{\Gamma}(\mathbf{Q})\hat{\chi}^{1D}(\mathbf{Q})]^{-1}\}_{11}$, and

$$\xi_x^2=\xi_y^2=2[12(b_0\chi_u^{1D}+b_Q\chi_s^{1D})c_Q\chi_s^{1D}+8b_Qc_0\chi_u^{1D}\chi_s^{1D} +16b_Q^2c_0\chi_u^{1D}(\chi_s^{1D})^2+80c_Q\chi_s^{1D}b_0b_Q\chi_u^{1D}\chi_s^{1D}] \times 1/(1-A_0), \quad (14)$$

$$\xi_z^2=[16(b_0\chi^{1D}+b_Q\chi_s^{1D})c_Q\chi_s^{1D}+32b_Qc_0\chi_u^{1D}\chi_s^{1D} +64b_Q^2c_0\chi_u^{1D}(\chi_s^{1D})^2+64c_Q\chi_s^{1D}b_0b_Q\chi_u^{1D}\chi_s^{1D}] \times 1/(1-A_0), \quad (15)$$

$$A_0=8(b_Q\chi_s^{1D}+b_0\chi_u^{1D})^2+16b_0b_Q\chi_u^{1D}\chi_s^{1D} +64(b_Q\chi_s^{1D}+b_0\chi_u^{1D})b_0b_Q\chi_u^{1D}\chi_s^{1D}, \quad (16)$$

with $\chi_u^{1D}=\chi_u^{1D}(q=0)$, $\chi_s^{1D}=\chi_s^{1D}(q=Q_0)$, $b_0=(zV/v_s)^2/(\pi v_F)$, $b_Q=(zV/v_s)^2\ln(4t/v_F\Delta k)/(\pi v_F)$, $c_0=4(zV/v_s)^2/(3\pi^2v_F)$, and $c_Q=(zV/v_s)^2/(16\pi v_F\Delta k^2)$. Using Eq. (13), we compute the self-energy Σ_{11} and obtain the mass enhancement factor,

$$-\frac{\partial\Sigma_{11}}{\partial\varepsilon}\sim\frac{192\sqrt{2}V^4\chi_0(\mathbf{Q})}{\pi^2v_s^2v_F\xi_y\xi_z}\ln\left[1+\left(\frac{\xi_y^2}{2}+\xi_z^2\right)\pi\right]\sim 4.33. \quad (17)$$

Then, we end up with the specific-heat coefficient,

$$\gamma=\left(1-\frac{\partial\Sigma}{\partial\varepsilon}\right)\frac{2\pi}{3v_F}\sim 222\ \ (\mathrm{mJ/mol\,K^2}). \quad (18)$$

This is almost consistent with experimentally observed values, i.e., $350\sim 420$ mJ/mol K^2. Since our approximation underestimates electron correlation effects, the above result gives a lower bound for γ.

V. SUMMARY AND COMMENTS

In this paper, we have proposed a microscopic scenario for the HF state of LiV_2O_4. It has been shown that magnetic, thermodynamic, and transport properties of LiV_2O_4 are well understood in terms of the Hubbard chains network model. In the high-temperature region, the system is in the 1D-like state showing anomalous transport properties. As temperature is lowered, the crossover to 3D Fermi-liquid state occurs. The origin of heavy-fermion mass is ascribed to en-

hanced electron correlation of the 1D-like structure.

The validity of our model completely relies on the assumption that the system is on the border of the dimensional crossover. We need more experimental tests to confirm the validity of our scenario. Very recently, Li-NMR measurement under ambient pressure has been carried out by Fujiwara *et al.*[27] They found that the spin-lattice relaxation rate $(T_1T)^{-1}$ increases, as the applied pressure is increased, showing the enhancement of the spin fluctuation. This behavior is quite different from that expected for usual strongly correlated metals like *f*-electron based HF systems. This experimental fact may be easily understood in terms of the dimensional crossover phenomena described by our model.

Finally, we make a brief comment on single-particle properties. It is known that in the 1D Hubbard model at quarter filling, v_c is much larger than v_s for large U. In our case $(U/4t=2)$, $v_c=1.9t$ and $v_s=0.6t$. Thus it is expected that for $T^*<T\ll E_F/k_B$ the single-particle spectrum have two peaks which correspond to charge and spin degrees of freedom, indicating spin-charge separation. It may be intriguing to search for spin-charge separation behavior in LiV_2O_4 by photoemission spectroscope experiment.

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