Model-mapped RPA to evaluate superconductivity in FLEX from first-principles

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We have applied the model-mapped RPA [H. Sakakibara et al., J. Phys. Soc. Jpn. 86, 044714 (2017)] to the cuprate superconductors La$_2$CuO$_4$ and HgBa$_2$CuO$_4$, resulting two-orbital Hubbard models. All the model parameters are determined based on first-principles calculations. For the model Hamiltonians, we perform fluctuation exchange calculation. Results are consistent with experimental $T_c$. In addition, we give some analyses for the interaction terms in the model, especially comparisons with those of the constrained RPA.

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-Introduction. It is not so easy to treat strongly-correlated electrons only by first-principles calculations. Thus we often use a procedure via a model Hamiltonian; we determine a model Hamiltonian $\hat{H}_M$ from a first-principles calculation and then solve the model Hamiltonian $[1, 2]$. This is inevitable because first-principles calculations, which are mainly based on the density functional theory (DFT) in the local density approximation (LDA), are very limited to handle systems with correlated electrons. Widely used model Hamiltonians are the Hubbard ones, which consist of one-body Hamiltonian $\hat{H}_M^0$ and the on-site interactions $\hat{U}_M$. To solve the Hubbard models, we can use a variety of methods such as fluctuation exchange approximation (FLEX) $[3, 11]$.

To determine $\hat{H}_M$, we have formulated the model-mapped random phase approximation (mRPA) in Ref. 12 recently. In mRPA, we use the standard procedure of the maximally localized Wannier function $[13, 14]$ to determine $\hat{H}_M^0$. Here $\hat{H}_M^0$ is determined as a projection of the one-body Hamiltonian of first-principles onto a model space, which is spanned by the Wannier functions. Then we determine $\hat{U}_M$ so that the screened interaction of the model in the random phase approximation (RPA) agrees with that of the first-principles. Then we determine one-body double-counting term $\hat{U}_M$. Finally we have $\hat{H}_M = \hat{H}_M^0 + \hat{U}_M - \hat{U}_M$. The constrained RPA (cRPA) $[12, 16]$ have also developed to determine $\hat{U}_M$ $[17, 31]$, however, mRPA is advantageous since mRPA is free from difficulties of cRPA. For example, a difficulty is that cRPA gives long-range model interaction unsuitable for Hubbard models, since cRPA removes all the metallic screenings. Furthermore, we need to remind that cRPA cannot be applied to metallic systems as it is $[12]$.

In this Rapid Communication, we apply mRPA to high-$T_c$ cuprate superconductors La$_2$CuO$_4$ ($T_c = 39$ K $[32]$, denoted by La) and HgBa$_2$CuO$_4$ ($T_c = 98$ K $[33]$, denoted by Hg) to determine $\hat{H}_M$ of a two-orbital model $[34, 37]$. After we determine $\hat{H}_M$, we perform FLEX calculations to investigate superconductivity. Our results are consistent with experiments. Since this mRPA+FLEX procedure can be performed without parameters by hand, we can claim that $T_c$ is evaluated just from crystal structures. Thus, in principle, mRPA+FLEX can be used to find out a highest $T_c$ material among a lot of possible materials.

We like to emphasize importance of the two-orbital model $[34, 37]$. Although the Fermi surface of cuprates consists of the $d_{x^2-y^2}$ orbital mainly, Sakakibara et al. pointed out that hybridization of the $d_{x^2-y^2}$ orbital with the $d_z$ orbital $[38, 52]$ is very important $[53]$. This can be represented by the two-orbital model. Sakakibara’s FLEX calculation showed that the hybridization degrades spin-fluctuation-mediated superconductivity. This explains the difference of $T_c$ between La and Hg cuprates $[34]$. A recent photoemission experiment for La cuprate has captured significant orbital hybridization effects $[54]$.

-Method. Let us summarize the formulation of mRPA in Ref. 12. First of all, we have to parametrize the interaction $\hat{U}_M$ of the model Hamiltonian so that $\hat{U}_M$ is specified by finite numbers of parameters. Fig. 1 is a chart about how we determine $\hat{U}_M$. Step (1) is by first-principles calculations, and step (2), (3) are by model calculations. In this Rapid Communication, we will treat the onsite-only interaction of the two-orbital model specified by four parameters.

In step (1) of Fig. 1 we first perform a self-consistent calculation in first-principles method. Then we can obtain one-body Hamiltonian $\hat{H}_M^0$ in the standard procedure of maximally localized Wannier function $[13, 14]$. In addition, we calculate a static screened Coulomb interaction $\hat{W}(\mathbf{r}, \mathbf{r}', \omega = 0)$ in RPA. Hereafter we omit $\omega = 0$ since we treat only the static case in this Rapid Communication. Then we calculate matrix elements $W^{11/22'}$ of the matrix $\hat{W}$, defined as

$$W^{11/22'} = \langle 11' | W | 22' \rangle$$

$$= \int d\mathbf{r} d\mathbf{r'} \phi_1^*(\mathbf{r})\phi_1(\mathbf{r}) W(\mathbf{r}, \mathbf{r'}) \phi_2(\mathbf{r'})\phi_2^*(\mathbf{r'})$$

where $\{\phi_1(\mathbf{r})\} = \{\phi_i(\mathbf{r})\}$ are the Wannier functions. $\mathbf{R}$ and $i$ denote a position of primitive cell and an or-
FIG. 1. How mRPA determines a model Hamiltonian \( \hat{H}_M \). Note that quantities with subscript \( M \) are for the model Hamiltonian. At step (1), we obtain one-body Hamiltonian \( H^0_M \) and RPA screened Coulomb interaction \( W^{11',22'}_M \) in a first-principles calculation. At step (2), we obtain effective interaction \( U_M \) in the model, where we require \( W^{11',22'}_M \) should be the same as \( W^{11',22'} \). At step (3), we determine \( \bar{U}_M \), which is to remove the double counting in the one-body term.

bital in each cell, respectively. The number of elements \( W^{11',22'}_M \) is the same as the number of elements \( U^{11',22'}_M \). Calculations are performed with ecalj package available from Git-hub [57].

In step (2), we determine \( U_M \), so that it satisfies

\[
W^{11',22'}_M [H^0_M, U_M] = W^{11',22'},
\]

where a functional \( W^{11',22'}_M [H^0_M, U_M] \) is a screened interaction in RPA calculated from \( H^0_M \) and \( U_M \). Here \( H^0_M \) denotes the matrix whose elements are \( H^0_M^{1,2} \); \( U_M \) denotes the matrix whose elements are \( U^{11',22'}_M \) as well. \( \bar{H}^0_M \) is the second quantized operator made of the matrix \( H^0_M \) in the model. The functional is defined just in the model calculation; we do not treat quantities spatially dependent on \( r \). Eq. (2) is a key assumption of mRPA; we require that the screened interaction in a model should be the same as those of theoretical correspondence in the first-principles calculation.

Let us detail the functional \( W^{11',22'}_M [H^0_M, U_M] \). With non-interacting polarization function \( P_M[H^0_M] \) of a model, we have effective interaction \( W_M \) in RPA as

\[
W_M[H^0_M, U_M] = \frac{1}{1 - U_M P_M[H^0_M]} U_M.
\]

Hereafter we omit \( H^0_M \) in \( P_M \) for simplicity. Here we only treat non-magnetic case. From Eq. (3), we have

\[
W^{i_1,i_2;i_1',i_2'}_M [H^0_M, U_M] = \frac{1}{N} \sum_q \left[ \frac{1}{1 - U_M P_M(q)} U_M \right]_{i_1,i_2;i_1',i_2'}.
\]

for on-site interactions \( U_M \) and \( W_M \). Eq. (4) is used in Eq. (2) so as to determine \( U_M \).

In step (3), we evaluate the one-body double counting term \( \bar{U}_M \) contained in the total model Hamiltonian \( \hat{H}_M \). It is written as

\[
\hat{H}_M = \hat{H}^0_M + \bar{U}_M - \bar{U}_M.
\]

To determine \( \bar{U}_M \), we require that the contribution from \( \bar{U}_M \) and that from \( \bar{U}_M \) completely cancel when we treat \( \bar{U}_M \) in a mean-field approximation. The mean-field approximation should theoretically correspond to the first-principle method from which we start. For example, if we use quasi-particle self-consistent GW (QSGW) [58-60] as the first-principle method, we have to use QSGW to treat the model of Eq. (3). Then \( \bar{U}_M \) is made of the Hartree term and the static self-energy term in the model. These terms cancel the effect of \( \bar{U}_M \) when QSGW is applied to. In this case, we have reasonable theoretical correspondence between the first-principle calculation and model calculation. However, if we use LDA as the first-principle method, we have no corresponding mean-field approximation. Thus we cannot uniquely determine \( \bar{U}_M \) instead of determining \( \bar{U}_M \), we use a practical method to avoid double counting in FLEX (see the FLEX part).

Recall that the computational procedure of cRPA is very different from that of mRPA. The effective interaction of cRPA \( U_m \) is determined based on the requirement

\[
\frac{1}{1 - v P} = \frac{1}{1 - U_m P_m} U_m,
\]

where \( v(r, r') \) is the bare Coulomb interaction, \( P_m(r, r') \) is the polarization function within the partial space spanned by the maximally localized Wannier function. This leads to

\[
U_m = \frac{1}{1 - v(P - P_m)} v.
\]

Then we calculate the on-site matrix elements \( U^{12';1'}_{m} \) \((11' |U_m| 22') \) cRPA is numerically more complicated than mRPA since we treat spatial dependence of \( P_m(r, r') \). In contrast, mRPA only treat \( P_m \) of a Hubbard model. In addition, we need some special treatments to keep positive definiteness of \(-v(P - P_m)\) in Eq. (7) in the metallic systems [12, 61, 62].

-Results. Following the chart of Fig. 1, we apply mRPA to single-layered cuprates, La and Hg, to obtain the two-orbital Hubbard model [34], where we start from LDA calculations. We show their experimental crystal structures [53, 56] in Fig. 2 together with their LDA band structures in (b) and (d), where we superpose the energy bands of the two-orbital models. In addition, we
treat hypothetical cases varying apical oxygen height $h_{O}$ in La, (a) and (c), in order to clarify differences between mRPA and cRPA. Here $h_{O}$ is defined as the distance shown in Fig. 2. The matrix $U_{M}$ of the two-orbital model is represented as

$$U_{M} = \begin{pmatrix}
U_{x} & U_{y} & 0 & 0 \\
0 & U_{y}' & U_{x}' & 0 \\
0 & 0 & U_{x}' & U_{y}' \\
U_{y}' & 0 & 0 & U_{x}'
\end{pmatrix}, \quad (8)$$

where indices of the four by four matrix $U_{M}$ takes the $d_{x^2-y^2}d_{z^2-y^2}$, $d_{x^2-y^2}d_{z^2}$, $d_{x^2}d_{z^2-y^2}$, and $d_{x^2}d_{z^2}$ orbitals. Here $U'$ is inter-orbital Coulomb interactions and $U^J = U^J$ are exchange interactions. Other interactions such as $W_{M}$ are represented as well.

**TABLE I.** The interactions of mRPA ($U_{M}$) and cRPA ($U_{m}$) for the experimentally observed crystal structure of La$_2$CuO$_4$ and HgBa$_2$CuO$_4$ [55, 56]. Static screened Coulomb interaction $W_{M}[U_{m}]$ is also shown (see text). The elements of $W$ are defined in the same manner as $U_{M}$.

| Compound   | mRPA | cRPA | $W_{M}[U_{m}]$ |
|------------|------|------|----------------|
| La$_2$CuO$_4$ | 2.76 | 3.14 | 0.747 | 0.769 |
| HgBa$_2$CuO$_4$ | 2.63 | 3.04 | 1.58 | 1.66 |
| U'         | 1.64 | 2.03 | 0.370 | 0.412 |
| U''        | 0.44 | 0.42 | 0.273 | 0.262 |

In Table I we show values of $U_{M}$ for La and Hg (Fig. 2(b) and 2(d)), together with values of $W$ [52]. We also show values of $U_{m}$ and $W_{M}[U_{m}]$, related to cRPA, and will discuss in a later paragraph. Most important elements are $U_{x^2-y^2}$ since the $d_{x^2-y^2}$ orbital is the main orbital at the Fermi surface. Table I shows $U_{x^2-y^2}$ are 2.76 eV (La) and 2.99 eV (Hg).

Let us show that $U_{x^2-y^2}$ is roughly estimated by

$$U_{x^2-y^2} \sim \frac{W_{x^2-y^2}}{1 + W_{x^2-y^2}P_{M}^{x^2-y^2}}, \quad (9)$$

where $P_{M}^{x^2-y^2}$ is the diagonal elements of the Brillouin zone average of $P_{M}(q)$. Eq. (9) is derived from Eq. (4) by replacing $P_{M}(q)$ with the average. Let us evaluate $P_{M}(q)$. Our calculation gives $P_{M}^{x^2-y^2} = 0.97$ eV$^{-1}$ for La, 0.91 eV$^{-1}$ for Hg. The little difference $0.06=0.97-0.91$ eV$^{-1}$ corresponds to the little difference of the band structures of the two-orbital models shown in Fig. 2(b) and 2(d).

Together with the values of $W_{x^2-y^2} = 0.747, 0.820$ eV in Table I, Eq. (9) gives $U_{x^2-y^2} \sim 2.64$ eV for La and $\sim 3.33$ eV for Hg. These are roughly in agreement with $U_{x^2-y^2} = 2.76$ and 2.99 eV in Table I. This analysis indicates that the difference of $U_{x^2-y^2}$ between La and Hg is mainly due to the difference of $W_{x^2-y^2}$.

In Table I we also show cRPA values $U_{m}$ together with $W_{M}[U_{m}]$ which denotes $W_{M}[H_{M}^{0}/U_{m}]$. Hereafter we skip $H_{M}^{0}$ for simplicity. $W_{M}[U_{m}]$ is calculated in the same manner as $W_{M}[U_{m}]$: the difference $W_{M}[U_{m}] - W$ can be taken as a measure of inconsistency of cRPA. Roughly speaking, we see agreements $U_{M} \sim U_{m}$. This is reasonable because both of mRPA and cRPA are conceptually on the same principle that screening effect due to polarization contained in a model should be removed. However, we see some discrepancies, especially in Hg, that $U_{m}^{x^2-y^2} = 2.14$ eV is very smaller than $U_{M}^{x^2-y^2} = 2.99$ eV. This can be because $P_{m}(r,r')$ in Eq. (4) is affected not only by energy bands, but also by the localization of the Wannier functions. When Wannier functions are more delocalized, we expect spatially more gentle screenings resulting less screening for on-site interactions. For a given value of $W(r,r')$ (left-hand side of Eq. (4)), less screening by $P_{m}(r,r')$ gives smaller $U_{m}(r,r')$. We expect more delocalized Wannier functions for higher $h_{O}$; $h_{O}$ is 2.41 Å for La, 2.78 Å for Hg [55, 56]. In Fig. 3 we illustrate how $h_{O}$ determines the localization.
FIG. 3. (Color online) This illustrates why higher $h_0$ gives less localization of the Cu-$d_{x^2−y^2}$ Wannier orbital. Left (right) panel shows that lower (higher) $h_0$ gives the larger (smaller) level-offset $\Delta_{dp}$ between the Cu-$d_{x^2−y^2}$ orbital and the O-$p_x,p_y$ orbitals due to the effect of the Madelung potentials from the apical oxygen. Smaller $\Delta_{dp}$ makes Cu-$d_{x^2−y^2}$ more hybridized with O-$p_x,p_y$. In other words, the Wannier functions of Cu-$d_{x^2−y^2}$ becomes more delocalized. In the bottom pictures, we illustrate the Wannier functions, where we show amounts of orbital components by their sizes.

varying $h_0$ in La. Let us focus on Fig. 4(a) and 4(e). As a function of $h_0$, $W^{x^2−y^2}$ is almost constant. In addition, the energy bands of the two-orbital model $\hat{H}_M^0$ (and hence $P_m(H_M^0)$) change little as shown in Fig. 2(a)-(c). Thus it is reasonable that $U_M^{x^2−y^2}$ changes little in 4(a), because of Eq. (9). On the other hand, $U_M^{d_{x^2−y^2}}$ decreases more rapidly than $U_M^{x^2−y^2}$ as $h_0$ becomes higher. This can be interpreted as the effect of delocalization of the Wannier functions, indicating less screening by $P_m(r,r')$ for higher $h_0$.

This rapid decrease of $U_M^{x^2−y^2}$ is shown in our previous paper of cRPA; we showed that higher $h_0$ gives smaller $U_M^{x^2−y^2}$ due to the less localization of the Wannier functions for a variety of layered cuprates [29]. The results of cRPA are in agreement with experiments. In contrast, we see very flat $U_M^{x^2−y^2}$ of mRPA as shown in 4(a). Considering the agreement in cRPA, this can be a problem of mRPA. However, our results presented in this Rapid Communication are limited to assess this problem. We need further systematic investigations in mRPA, especially, need to treat bigger models including off-site interactions [64].

-FLEX calculation for superconductivity. For the model Hamiltonian $\hat{H}_M$ obtained from mRPA, we perform two-orbital FLEX calculation to obtain dressed Green’s functions $G_{ij}(k)$ [3, 65–67]. Here $k = (k, i\omega_n)$ is a composite index made of the wave vector $k$ and the Matsubara frequency $i\omega_n$. We calculate only the optimally doped case for $T_c$ (15% doping). We take $32 \times 32 \times 4$ k-meshes and 1024 Matsubara frequencies.

Since we start from LDA, we have no unique way to determine $U_M$ as we discussed in the method part. Here we identify the static part of the self-energy $\Sigma(k,0)$, including the Hartree term, as $\bar{U}_M$. Thus the static part is fixed by the LDA calculations. This method is introduced at Eq. (5) in Ref. [68]. In practice, we subtract the self-energy at lowest Matsubara frequency $\text{Re}\Sigma(k, i\omega_n=0)$. We take $15\%$ doping. We calculate only the optimally doped case for $T_c$ (15% doping). We take $32 \times 32 \times 4$ k-meshes and 1024 Matsubara frequencies.

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Next, we investigate superconductivity in the two-orbital model. By substituting $G_{ij}(k)$ into the linearized Eliashberg equation,

$$\lambda\Delta_{ij}(k) = -\frac{T}{N} \sum_{q,m_1} V_{m_1,m_2}(q) G_{m_1,m_2}(k−q) \times \Delta_{m_2,m_3}(k−q) G_{m_3,m_4}(−k+q),$$

we obtain the gap function $\Delta_{ij}(k)$ as an eigenstate and its
FIG. 5. (Color online) The eigenvalues $\lambda$ of the Eliashberg equation are plotted as a function of $U^{x^2-y^2}$. Here the temperature is 0.01 eV. Red filled circles show the value for La and blue squares for Hg. Open circles indicate the results obtained with the value shown in table I.

eigenvalue $\lambda$, where $V(q)$ is the singlet pairing interaction as described in Eq. (2)-(7) of Ref. 33. $\lambda$ reaches unity at $T = T_c$. Since $\lambda$ is monotonic and increasing function of $T^{-1}$, we use $\lambda$ at $T = 0.01$ eV as a qualitative measure of $T_c$ instead of calculating at $T_c$. We obtain $\lambda = 0.50$ for La and 0.71 for Hg. This is consistent with the experimental observation, where $T_c = 39$ K for La and $T_c = 98$ K for Hg 32, 33.

To investigate how $U_M$ affects $\lambda$ in more detail, we perform calculations by rescaling $U_M$ hypothetically. We plot $\lambda$ as a function of $U^{x^2-y^2}$ in Fig. 2. In the calculation, $U_M^0$ and the ratio between all the elements of $U_M$ are fixed. We see that $\lambda$ increases rapidly with smaller $U^{x^2-y^2}$ and plateaus with larger $U^{x^2-y^2}$ in both materials 33. The cases of original $U^{x^2-y^2}$ as shown in table I are shown by open circles. These are in the plateau region 70. Because of the small changes in the region, $\lambda$ of the two cuprates do not change so much even if we use $U_m$ instead of $U_M$, where $\lambda_{\text{La}}^{\text{cRPA}} = 0.52$ and $\lambda_{\text{Hg}}^{\text{cRPA}} = 0.64$. The difference between La and Hg is mainly from the hybridization of the $d_{x^2-y^2}$ orbital with the $d_{z^2}$ orbital. This is already examined by previous FLEX calculations with empirically determined interaction parameters 34. Sakakibara et al. already showed that FLEX reproduces the experimental trends of $T_c$ (see Fig. 1(a) of Ref. 34). The detailed mechanism how the hybridization affects $T_c$ was discussed in Sec. III D of Ref. 34.

Summary. With mRPA, we obtain the two-orbital Hubbard models for La$_2$CuO$_4$ and HgBa$_2$CuO$_4$ in first-principles. The main part of mRPA is how to determine the on-site interaction parametrized by four parameters. We see that the interactions are close to those in cRPA. However, we see some differences. A difference comes from the fact that mRPA does not include localization effects of 3$d$ electrons via the polarization function. This is because that the polarization function of the model is determined only by one-body Hamiltonian.

For the models, we perform FLEX to evaluate superconductivity. The results are consistent with experiments. With the interaction obtained in mRPA, we confirm that $T_c$ is not so strongly dependent on the scale of interaction. Along the line of the combination of mRPA and FLEX, we will be able to predict new superconductors.

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