Quantum Monte Carlo study of the pairing symmetry competition in the Hubbard model

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To shed light into the pairing mechanism of possible spin-triplet superconductors (TMTSF)\textsubscript{2}X and Sr\textsubscript{2}RuO\textsubscript{4}, we study the competition among various spin singlet and triplet pairing channels in the Hubbard model by calculating the pairing interaction vertex using the ground state quantum Monte Carlo technique. We model (TMTSF)\textsubscript{2}X by a quarter-filled quasi-one dimensional (quasi-1D) Hubbard model, and the \(\gamma\) band of Sr\textsubscript{2}RuO\textsubscript{4} by a two dimensional (2D) Hubbard model with a band filling of \(\sim 4/3\). For the quasi-1D system, we find that triplet \(f\)-wave pairing not only dominates over triplet \(p\)-wave in agreement with the spin fluctuation theory, but also looks unexpectedly competitive against \(d\)-wave. For the 2D system, although the results suggest presence of attractive interaction in the triplet pairing channels, the \(d\)-wave pairing interaction is found to be larger than those of the triplet channels.

I. INTRODUCTION

Possible occurrence of spin-triplet pairing in superconductors such as a ruthenate Sr\textsubscript{2}RuO\textsubscript{4} and organic materials (TMTSF)\textsubscript{2}X (X=ClO\textsubscript{4}, PF\textsubscript{6} \ldots) has attracted much attention lately. A probable mechanism of spin-triplet pairing is due to ferromagnetic spin fluctuations, as in \(^3\)He, as proposed in ref.\textsuperscript{7} for Sr\textsubscript{2}RuO\textsubscript{4}. In both of these materials, however, the mechanism of triplet pairing has been controversial because the spin fluctuation has turned out to be more like antiferromagnetic than ferromagnetic. Namely in (TMTSF)\textsubscript{2}X, the nesting of the quasi-1D Fermi surface give rise to a \(2k_F\) spin density wave phase lying right next to the superconducting phase. In Sr\textsubscript{2}RuO\textsubscript{4}, spin fluctuations with a wave number \((2\pi/3, 2\pi/3)\) arises due to the nesting of the quasi-1D \(\alpha\) and \(\beta\) bands.

For (TMTSF)\textsubscript{2}X, the possibility of spin triplet \(p\)-wave pairing has been considered from the early days\textsuperscript{9,10,11}, but if we consider the \(2k_F\) spin fluctuations to be the origin of the pairing interaction, spin singlet \(d\)-wave-like pairing is more likely to occur as proposed by several authors.\textsuperscript{12,13,14,15} Recently, two of the present authors have proposed, based on a phenomenological spin-fluctuation theory, that a combination of quasi-one-dimensionality, the coexistence of \(2k_F\) spin and charge fluctuations, and anisotropy in the spin fluctuations may lead to spin-triplet \(f\)-wave pairing, dominating over \(d\)- and \(p\)-wave pairings.\textsuperscript{16} A similar proposal has been made by Fuseya et al.\textsuperscript{17} In fact, the coexistence of \(2k_F\) spin and charge density wave has been reported experimentally\textsuperscript{18,19}. However, a recent renormalization group study by Fuseya et al\textsuperscript{16} has suggested that \(p\)-wave pairing dominates over \(f\)-wave pairing in quasi-1D systems.

For Sr\textsubscript{2}RuO\textsubscript{4} on the other hand, there has been a debate as to which one of the three bands plays the main role in the occurrence of superconductivity, namely the 2D \(\gamma\) bands or the quasi-1D \(\alpha\)-\(\beta\) bands. Several microscopic theories have focused on the antiferromagnetic spin fluctuations due to the \(\alpha\)-\(\beta\) band Fermi surface nesting.\textsuperscript{21,22} In refs.\textsuperscript{21,22} in particular, the experimentally observed anisotropy in the spin fluctuations is the key for spin-triplet \(p\)-wave pairing to take place.

On the other hand, Nomura and Yamada focused mainly on the 2D \(\gamma\) band.\textsuperscript{27} Applying third order perturbation theory to the 2D Hubbard model with appropriate band structure and band filling, they showed that triplet pairing superconductivity takes place, dominating over singlet pairing. A multiband calculation has recently been performed along this line.\textsuperscript{28} Also, a renormalization group study has been performed for the Hubbard model having nearest neighbor hopping, where spin triplet pairing is shown to be the leading instability near but away from the van Hove filling.\textsuperscript{29} By contrast, if we apply random phase approximation (RPA) type theories like the fluctuation exchange method (FLEX)\textsuperscript{30} to the 2D Hubbard model, triplet pairing not only does not occur in a realistic temperature regime\textsuperscript{31,32} but also does not even dominate over singlet pairing at the filling corresponding to the \(\gamma\) band of Sr\textsubscript{2}RuO\textsubscript{4} (see section V D).

The purpose of the present study is to shed light into these controversies. We model (TMTSF)\textsubscript{2}X and Sr\textsubscript{2}RuO\textsubscript{4} by quasi-1D and 2D Hubbard models, respectively. Using the ground state quantum Monte Carlo technique, we calculate the pairing interaction vertices for possible pairing symmetries.
Fermi surface. In the case of (TMTSF)_2X, two disconnected pieces of the quasi 1D Fermi surface are separated by the nesting vector $Q$. The transfer arrows denote a pair scattering process having a momentum transfer $Q$.

Before going into the QMC calculation, here we summarize the spin-charge fluctuation theory of quasi-1D systems given in ref.16. The pairing interactions mediated by spin and charge fluctuations are generally given as

$$V_{\alpha}(q) = \frac{1}{2} V_{\alpha}^{zz}(q) + V_{\alpha}^{+/-}(q) - \frac{1}{2} V_{\alpha}(q)$$

for singlet pairing,

$$V_{\perp}(q) = -\frac{1}{2} V_{\perp}^{zz}(q) - \frac{1}{2} V_{\perp}(q)$$

for triplet pairing with total $S_z = \pm 1$ ($d$-vector $d \perp z$), and

$$V_{||}(q) = \frac{1}{2} V_{||}^{zz}(q) - V_{||}^{+/-}(q) - \frac{1}{2} V_{||}(q)$$

for triplet pairing with $S_z = 0$ ($d || z$). Here $V_{\alpha}^{zz}$, $V_{\alpha}^{+/-}$, and $V_{\alpha}$ (all positive) are contributions from the longitudinal spin, transverse spin, and charge fluctuations, respectively. We assume that the fluctuations are enhanced at $q = Q$, where $Q$ is the nesting vector of the Fermi surface. In the case of (TMTSF)_2X, $Q$ bridges the two disconnected pieces of the quasi 1D Fermi surface (see Fig.1). The pairing symmetry is determined so as to make the quantity

$$V_{\text{eff}} = -\sum_{k,k' \in \text{Fermi surface}} V_{\alpha}(k-k')\phi(k)\phi(k')$$

positive and large, where $V_{\alpha}(k-k')$ is one of the pairing interactions (1)-(3) and $\phi(k)$ is the gap function. When $V_{\alpha}(q)$ peaks around the nesting vector $q = Q$, the contribution around $k - k' = Q$ becomes dominant in the summation of eqn. (4), so that the sign of the quantity $V_{\alpha}(Q)\phi(k)\phi(k + Q)$ has to be negative in order to have superconductivity.

Let us now consider $p$, $d$, $f$-wave gap functions shown in Fig.2 along with the Fermi surface. Although the $d$- ($f$-) wave gap is not $d$ ($f$) in the strict sense of the word, here we use this terminology in the sense that the gap changes sign as $++ --$ along the Fermi surface. Since the $d$-wave gap function satisfies $\phi(k)\phi(k + Q) < 0$, a positive pairing interaction $V_{\alpha}(Q)$ is necessary for superconductivity to occur in this channel. Similarly $V_{\perp}(Q) < 0$ or $V_{||}(Q) < 0$ is necessary for $f$-wave pairing. If we assume $V_{zz}^{sp} \geq V_{sp}^{+/-}$, $|V_{\perp}(Q)| > |V_{||}(Q)|$, so that $f$-wave is more likely to occur in the $d \perp z$ channel. Since the number of nodes of the gap intersecting the Fermi surface is the same between $d$ and $f$ due to the quasi-one-dimensionality, the competition between the two is almost solely dominated by the absolute value of the pairing interaction. Thus the boundary between $d$ and $f$-waves is roughly given by $V_{\perp}(q) = -V_{\alpha}(q)$, which corresponds to the line $V_{ch} = V_{zz}^{sp}$. In particular, when the system has spin rotational symmetry, the two symmetries become nearly degenerate when spin and charge fluctuations have about the same strength.

On the other hand, the $p$-wave gap function satisfies $\phi(k)\phi(k + Q) < 0$, so that a positive triplet pairing interaction is necessary. This can be the case only for $d \parallel z$ and only when $V_{ch}/V_{zz}^{sp}$ and $V_{sp}^{+/-}/V_{zz}^{sp}$ are both small. Since the $p$-wave gap function is nodeless on the Fermi surface as opposed to the case of $d$- and $f$-waves, this will be the dominant pairing if the pairing interaction is positive and strong enough.

From the above phenomenological argument, we obtain a generic phase diagram given in Fig.2.

![Fig. 1](image1.png)

**FIG. 1:** $p$, $d$, and $f$-wave gap functions along with the Fermi surface of the quasi 1D system and the nesting vector $Q$. The arrows denote a pair scattering process having a momentum transfer $Q$.

![Fig. 2](image2.png)

**FIG. 2:** A generic phase diagram for quasi-1D systems.

### II. Spin-Charge Fluctuation Theory

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for triplet pairing with total $S_z = \pm 1$ ($d$-vector $d \perp z$), and

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From the above phenomenological argument, we obtain a generic phase diagram given in Fig.2.

### III. Formulation of the QMC Study

In this section, we formulate the ground state QMC study.
A. On-site Hubbard model

As a model for (TMTSF)$_2$X, we consider the Hubbard model

\[ H = - \sum_{\langle i,j \rangle} t_{ij} (c^\dagger_{i\sigma} c_{j\sigma} + c^\dagger_{j\sigma} c_{i\sigma}) + U \sum_i n_{i\uparrow} n_{i\downarrow} \]

on an $N_x \times N_y$ quasi-1D lattice shown in Fig. 3(a). We set $t_x \ll t_y$, where $t_x$ (taken as unity throughout the study) and $t_y$ are hopping integrals in the $x$ and $y$ directions, respectively. Since the energy band is much more dispersive in the $x$ direction than in the $y$ direction, we take more sites in the former than in the latter ($N_x \gg N_y$). As for the electron-electron interaction, we assume only the on-site repulsion $U$ for simplicity, and refer to the model as the on-site Hubbard model. The reason for this is to make the QMC calculation feasible. Note that, $U$ enhances only the spin fluctuation \( V_{sp}^{zz} = V_{sp}^{+-} \gg V_{ch} \), so that $d$-wave pairing is expected from the spin fluctuation theory\(^{12,13}\) as seen from the phase diagram. We take $U = 2$ throughout the study.

The band filling $n = (\text{number of electrons } N_e / \text{number of sites } N)$ is taken close to quarter filling, i.e., $n \simeq 0.5$.

As for Sr$_2$RuO$_4$, we focus on the $\gamma$ band and model it by the 2D single band Hubbard model having nearest and next nearest neighbor hoppings, $t$ and $t'$ respectively, as shown in Fig. 3(b). $t'$ has been estimated to be 0.3-0.4 in units of $|t|$.\(^{33,34,35}\) Here we take $t' = 0.4$. The band filling is taken to be close to $n = 4/3$.

B. Calculation conditions

We adopt the auxiliary field quantum Monte Carlo method for the ground state\(^{37,38,39,40}\). In this formalism, physical quantities are evaluated using the ground state wave function obtained as

\[ \exp(-\tau H) \langle \phi_T \rangle, \]

where $H$ is the Hamiltonian, $\tau$ is a sufficiently large number, and $\langle \phi_T \rangle$ is a trial state. $\tau$ is sliced into a product of many $\Delta \tau$ using Trotter-Suzuki decomposition\(^{40}\). In the actual calculation, we have taken $\beta \sim 10$, and $\Delta \tau \leq 0.1$, which turns out to be sufficient for a relatively small value of $U = 2$. The correlation functions are evaluated as the average of the calculation results of about 10 independent Monte Carlo runs, each of which consists of few thousand
MC sweeps. The error bars are estimated as the variation of the independent runs.

C. Pairing interaction vertex

We calculate the pairing interaction vertex for possible pairing channels \( \alpha \) which is defined as

\[
\Delta P_\alpha(i, j) = \sum_{\delta, \delta'} g_\alpha(\delta) g_\alpha(\delta') \times \\
\left\{ \left[ \langle c_{i, \delta} c_{i+\delta, j}^\dagger c_{j+\delta', j}^\dagger \rangle - \langle c_{i, \delta} c_{j+\delta', j}^\dagger c_{j+\delta', j}^\dagger \rangle \right] \\
\pm \left[ \langle c_{i, \delta} c_{i+\delta, j}^\dagger c_{j+\delta', j}^\dagger \rangle - \langle c_{i, \delta} c_{j+\delta', j}^\dagger c_{j+\delta', j}^\dagger \rangle \right] \\
\pm \left[ \langle c_{i, \delta} c_{i+\delta, j}^\dagger c_{j+\delta', j}^\dagger \rangle - \langle c_{i, \delta} c_{j+\delta', j}^\dagger c_{j+\delta', j}^\dagger \rangle \right] \\
+ \left[ \langle c_{i, \delta} c_{i+\delta, j}^\dagger c_{j+\delta', j}^\dagger \rangle - \langle c_{i, \delta} c_{j+\delta', j}^\dagger c_{j+\delta', j}^\dagger \rangle \right] \right\}
\]

Here, the signs \( \pm \) corresponds to singlet pairing, and \( - \) for triplet. \( g_\alpha(\delta) \) gives sign that depends on the pairing channel \( \alpha \) as given above. A positive interaction vertex in a certain pairing channel implies that there is an effective attractive pairing interaction in that channel between the renormalized quasi-particles.

For the quasi-1D system, we consider the pairing channels \( p_1, p_2, d \) and \( f \) as shown in Fig. 4(a) along with the signs \( g_\alpha(\delta) \). It can be easily shown that the corresponding gap functions in momentum space are proportional to \( \sin(2k_x) \), \( \sin(k_x) \), \( \cos(2k_x) \), and \( \cos(k_x) \), respectively. For the 2D system, three triplet pairings \( t_1, t_2, t_3 \) and a singlet pairing \( s_1 \) are considered as shown in Fig. 4(b). The corresponding gap functions in momentum space are proportional to \( \sin(k_x) \) (or equivalently \( \sin(k_y) \)), \( \sin(k_x + k_y) \) (or \( \sin(k_x - k_y) \)), \( \sin(2k_x) \) (or \( \sin(2k_y) \)), and \( \cos(k_x) - \cos(k_y) \), respectively. \( s_1 \) is the so-called \( d_{x^2-y^2} \) pairing.

Let us denote the \( i \)-th site as \( i = (i_x, i_y) \). For the 1D system, we calculate

\[
\Delta P_\alpha(r) = \sum_{iy} \Delta P_\alpha(i_x, i_y, j_x, j_y)
\]

(pairing correlation within each chain) as a function of distance in the \( x \) direction \( r = |i_x - j_x| \). For the 2D system, we calculate

\[
\Delta P_\alpha(r) = \sum_{i_x + iy = r} \Delta P_\alpha(i_x, i_y, j_x, j_y)
\]

as a function of the “distance” \( r \). In both systems, we focus on the long range part \( \Delta P_\alpha(r) \) because superconductivity is characterized by the long ranged behavior of the pairing correlation function.

D. Open shell and closed shell fillings

Since the energy scale of superconductivity in repulsively interacting systems is small, pairing correlations are known to be strongly affected by the energy level spacing around the Fermi level in finite size systems. Namely, since superconductivity occurs due to pair scattering between states near the Fermi level, the enhancement of the pairing correlation can be wiped out when the energies of the highest occupied levels and the lowest unoccupied levels are well separated.

In order to cope with this problem, here we consider the following two situations. (i) Open shell fillings: the number of electrons are chosen so that the \( k \)-points at the Fermi level is half-filled for the \( U = 0 \) ground state. The highest occupied and the lowest unoccupied states have the same energy in this case. We tune the value of the hopping integrals (\( t_y \) for the quasi-1D system and \( t \) for the 2D system) appropriately so as to distribute the \( k \)-points having the same energy as uniformly as possible along the Fermi surface.

In the case of open shell fillings, the trial state is chosen as follows. The \( U = 0 \) single particle states \( \exp(i \mathbf{k} \cdot \mathbf{r}) \) below the Fermi energy is completely filled with electrons. At the Fermi energy, the states of the form \( \exp(i \mathbf{k} \cdot \mathbf{r}) + \exp(-i \mathbf{k} \cdot \mathbf{r}) \) are filled only by up spin electrons, while the states of the form \( \exp(i \mathbf{k} \cdot \mathbf{r}) - \exp(-i \mathbf{k} \cdot \mathbf{r}) \) are filled only by down spin electrons. We will use gray circles to denote the half-filled \( k \)-points in the trial state, as shown in the inset of Figs. 4(b) and 10(a).

(ii) Closed shell fillings: the number of electrons is chosen so that the Fermi energy for the \( U = 0 \) ground state comes in between slightly separated energy levels. For the quasi-1D system, \( t_y \) is tuned so that the energy difference between the highest occupied and the lowest unoccupied levels is within 0.01\( t_x \) for \( U = 0 \). As for the 2D system, \( t_y \) is taken to be slightly different from \( t_x \) thereby lifting the degeneracy, by less than 0.01\( t_x \), between the highest occupied levels \( \mathbf{k} = (k_1, k_2) \) and the lowest unoccupied levels \( \mathbf{k} = (k_2, k_1) \).

In this case we take the \( U = 0 \) ground state, which is a state with total spin \( S_{tot} = 0 \), as the QMC trial state. Closed (open) circles will be used to denote the occupied (unoccupied) \( k \)-points that lie within 0.01\( t_x \) to the Fermi energy in the trial state, as shown in the inset of Figs. 4(b) and 10(b).

For open shell fillings, triplet pairing is expected to be favored because the electrons at the half-filled Fermi level tends to be in a high spin configuration. For closed shell fillings on the other hand, spin singlet pairing should be favored since we restrict ourselves to \( S_{tot} = 0 \) states by choosing the \( U = 0 \) ground state as the trial state. This problem does make the study of singlet-triplet competition less conclusive, but our results still give significant information concerning the \( d \)- vs. \( f \)-wave competition in the on-site Hubbard model as we shall see below. As for the competition within triplet pairings (\( p \) vs. \( f \)) on the other hand, we can safely give a robust conclusion.
IV. RESULTS AND DISCUSSIONS FOR THE QUASI 1D SYSTEM

A. Open shell filling

We now show the results for the quasi 1D system. We first present results for open shell fillings. The pairing interaction vertices $\Delta P_s$ are shown for three different sets of parameters in Fig. 4. In all cases, $\Delta P_f$ is found to be positive at large distances, while $\Delta P_{p1}$ and $\Delta P_{p2}$ are negative at most of the distances. This means that the spin-triplet pairing interaction is attractive in the $f$-wave channel and repulsive in the $p$-wave channels. This result is in contrast with the recent renormalization group study, and is at least qualitatively consistent with the spin-charge fluctuation theory described in section II, where $V_{sp}^z = V_{sp}^+ > V_h$, and thus $V_{sp}(Q) = V_{sp}(Q) < 0$ hold for the on-site Hubbard model.

The interaction vertex for $d$-wave pairing $\Delta P_d$ takes both positive and negative values, and we find $\Delta P_f > \Delta P_d$ at most of the large distances. This is somewhat surprising because when the system has spin rotational symmetry, $f$-wave can be competitive against $d$-wave only when $2k_F$ spin and $2k_F$ charge fluctuations have about the same strength as far as the spin-charge fluctuation theory concerned, which is not the case for the on-site Hubbard model.

As mentioned before, open shell filling is expected to favor spin triplet pairing, so this result may be regarded as an artifact due to the open shell filling. However, as we shall see later, open shell filling does not necessarily result in $\Delta P_{triplet} > \Delta P_{singlet}$. Another possible reason for $f$ dominating over $d$ is that effects beyond RPA-type theories may be important in quasi-1D systems. This is highly probable because Fermi liquid picture is known to be invalid at least in purely 1D systems.

B. Closed shell filling

Calculation results for a closed shell filling is shown in Fig. 4. In this case, we have positive $\Delta P_d$, smaller but still positive (or non-negative) $\Delta P_f$ for all distances, and clearly negative $\Delta P_p$. Thus, we may conclude that $\Delta P_f > \Delta P_p$ holds for both open and closed shell fillings. On the other hand, although the result of $\Delta P_d > \Delta P_f$ apparently seems to be consistent with the spin fluctuation theory, this result may not be taken directly is since closed shell fillings selectively favors spin singlet pairing as mentioned above. We shall come back to this point later.

V. RESULTS AND DISCUSSIONS FOR THE 2D SYSTEM

A. Open shell fillings

Let us now move on to the 2D system with $n \simeq 4/3$. We first look into the case with open shell fillings. In Fig. 7(a), we focus on the interaction vertices for triplet pairings, where we find positive interaction vertices for all three channels. However, if we compare singlet and triplet channels in Fig. 7(b), $\Delta P_{p1} > \Delta P_{p1}$ holds for all three triplet channels. A similar result is obtained also for a $14 \times 14$ system as seen in Fig. 8. Since the pairing forms are not optimized and there is a possibility of stronger triplet pairings between more separated sites than we have considered, we cannot conclude that singlet dominates over triplet. However, considering the fact...
that this is a result for an open shell filling, we may say that $d_{xz-y^2}$-wave is still a strong candidate for the most dominant pairing channel even though the band filling is considerably away from half filling and $t'$ is large.

This result provides an example of singlet pairing vertex being larger than that of the triplet pairings even for an open shell filling, which conversely supports our argument in section III A that $\Delta f > \Delta P_d$ in the quasi-1D system may not simply be an artifact of the open shell filling, and that $f$-wave may be competitive against $d$-wave even in the on-site Hubbard model due to effects beyond RPA-type theories.

B. Closed shell filling

In Fig.6 we present results for a closed shell filling. The interaction vertex for $sp_1$ pairing becomes larger than for the open shell filling (Fig.7). The vertices for triplet pairings this time take negative values for most of the distances. This is in contrast with the result for the quasi 1D system in Fig.5, where $\Delta f$ remains positive even for a closed shell filling. This comparison further enforces our argument that $f$-wave pairing is indeed a favorable pairing in the quasi-1D system.

C. Near full filling

To make sure that we have been on the right track, we present here QMC results for a nearly full filled (dilute hole density) case, where the outcome can be safely predicted. Namely in this case, spin triplet pairing is expected to dominate strongly over singlet since ferromagnetic spin fluctuations arise for $t' \sim 0.5$ and $n \sim 2$ (or equivalently $t' \sim -0.5$ and $n \sim 0$) due to the large density of states at the Fermi level. This can be considered as well established because a number of approaches, including a FLEX study,14 perturbational studies,49,50 a $T$-matrix approximation,51 and a renormalization group study,29 reach (at least qualitatively) the same conclusion in this parameter regime.

Since pairs may be formed at large distances for dilute career density, here we calculate the pairing interaction vertex also for the singlet $sp_3$ channel shown in the inset of Fig.10(b). For an open shell filling, the interaction vertices are in fact positive for all three triplet channels, while they are small or negative for the singlet $sp_1$ and $sp_3$ channels as seen in Fig.10(a). By contrast, for a closed shell filling, although the interaction vertices for $tp_1$ and $tp_3$ remains positive, they are much smaller than that for the singlet $sp_3$ channel. This result contradicts with the established result, again supporting our argu-
moment that the result $\Delta P_d > \Delta P_f$ for a closed shell filling in the quasi 1D system (Fig.7) may not be taken directly.

D. Comparison with FLEX

To close this section, we present FLEX calculation results for the 2D on-site Hubbard model with $n = 4/3$, $t' = 0.4$ and $U = 4$, and compare them with the QMC results given above. The formulation is as follows. First, the renormalized Green’s function is obtained within the FLEX method, which is kind of a self-consistent RPA. Secondly, the pairing interaction mediated by spin fluctuations is calculated within the RPA form. Finally, the FLEX Green’s function and the pairing interaction are substituted for the linearized Eliashberg equation, which is solved using the power method to give the largest eigenvalue and the corresponding eigenfunction (the gap function).

The gap functions having the largest eigenvalues are shown in Fig.11 for (a) the triplet and (b) the singlet pairing channels. The singlet gap function has a form close to $\cos(k_x) - \cos(k_y)$, which corresponds to sp1 pairing in the QMC study, while the form of the triplet gap function is close to $\sin(k_x + k_y)$, which corresponds to tp2. Although the eigenvalues are small (less than 0.3 for $T \geq 0.005$) for both singlet and triplet, the ratio between the singlet and triplet eigenvalues turns out to be $\lambda_{\text{singlet}}/\lambda_{\text{triplet}} \simeq 5$ at $T = 0.005$, which is at least qualitatively consistent with the QMC results.

VI. SUMMARY

To summarize, we have studied the competition among various pairing symmetries in the quasi-1D and the 2D on-site Hubbard models by calculating the pairing interaction vertices using the ground state QMC technique. For the quasi-1D system, $f$-wave pairing not only domi-
nates over \( p \)-wave in agreement with the spin-charge fluctuation theory, but also looks competitive against \( d \)-wave pairing. \( f \)-wave being competitive against \( d \)-wave in the on-site Hubbard model is rather unexpected from the spin-charge fluctuation theory because \( 2k_F \) charge fluctuation is not enhanced in the on-site Hubbard model.\(^{26}\)

If \( f \)-wave is competitive against \( d \)-wave even in the absence of strong charge fluctuations, it is likely that \( f \)-wave dominates over \( d \)-wave in the actual (TMTSF)\(_{2}X\), where \( 2k_F \) CDW actually coexists with SDW.\(^{13,19}\)

For the 2D system, the calculation results (at least for the open shell filling) support presence of attractive interaction in the triplet pairing channel. However, singlet \( d_{x^2-y^2} \) pairing dominates over all the triplet pairings considered in the present study at the band filling \( n \simeq 4/3 \), which corresponds to \( \text{Sr}_2\text{RuO}_4 \), in agreement with the FLEX calculation. Although we cannot completely rule out the possibility of other (longer ranged) triplet pairings dominating over singlet, or a possibility of triplet dominating over singlet for larger system sizes and/or larger values of \( U \), the present results do suggest that it is worth considering effects beyond the single band Hubbard model, including the contributions from the \( \alpha - \beta \) bands.\(^{21,22,23,24,25}\) in order to fully understand the occurrence of triplet superconductivity in \( \text{Sr}_2\text{RuO}_4 \).

Numerical calculation has been performed at the facilities of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo, and at the Computer Center, University of Tokyo.

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