Dynamical magnetic susceptibility in the lamellar cobaltate superconductor 
Na$_2$CoO$_2$.yH$_2$O

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I. INTRODUCTION

The spin dynamics in unconventional non $s$-wave superconductors is of fundamental interest due to its interesting and peculiar properties. This includes a non-trivial behavior of the magnetic part of the Knight shift in the spin-triplet superconductors, as well as an emergence of the so-called resonance peak observed in superconducting layered cuprates, which possesses spin-singlet $d_{x^2-y^2}$-wave order parameter symmetry. Furthermore, magnetic excitations are also often considered as a possible glue for the Cooper-pairing in a number of heavy-fermion and transition metal oxides compounds.

An analysis of the feedback effect of superconductivity on the magnetic spin susceptibility can be used to determine the symmetry of the superconducting order parameter. This is of particular significance for recently discovered water intercalated sodium cobaltate superconductor Na$_2$CoO$_2$.yH$_2$O, where the origin of superconductivity as well as an underlying symmetry of the superconducting order parameter is currently under debate. The studies of the specific heat and the $\mu$SR measurements of a magnetic penetration depth have revealed a line of nodes in the superconducting gap function $\Delta_K$. Similar conclusion has been made based on the measurements of the spin-lattice relaxation rate $1/T_1T$ by means of Nuclear Quadrupole Resonance (NQR), where absence of the characteristic Hebel-Slichter peak and power-law decrease upon decreasing temperature has been observed. Simultaneously, the developing of the strong antiferromagnetic (AFM) fluctuations above superconducting transition temperature, $T_c$, have been found. At the same time, early reports on the Knight shift’s temperature dependence, $K(T)$, have suggested a spin-triplet symmetry of the superconducting gap. In these Nuclear Magnetic Resonance (NMR) experiments, $K(T)$ was shown to be anisotropic for external magnetic field applied parallel or perpendicular to the $ab$-plane. In particular, $K_c(T)$ component has not shown a substantial decrease below $T_c$. This behavior has been interpreted in favor of the odd-parity Cooper-pairing in sodium cobaltate. Moreover, the most recent NMR experiments with higher precision have found a reduction of both Knight shift components as a function of temperature for $T < T_c$. These experiments points towards spin-singlet Cooper-pairing.

From the group-theoretical analysis the even-parity symmetries of the lowest harmonics for the triangular lattice are classified to $s$-wave ($\Delta_k = \Delta_0$), extended-$s$-wave ($\Delta_k = 2/3\Delta_0[\cos k_y + 2\cos (k_x\sqrt{3}/2) \cos (k_y/2)]$), $d_{x^2-y^2}$-wave ($\Delta_k = \Delta_0[\cos k_y - \cos (k_x\sqrt{3}/2) \cos (k_y/2)]$), $d_{xy}$-wave ($\Delta_k = \Delta_0[\sqrt{3}\sin (k_x\sqrt{3}/2) \sin (k_y/2)]$, and $d_{x^2-y^2} + id_{xy}$-wave representations. For both $d_{x^2-y^2}$- and $d_{xy}$-wave symmetries $\Delta_k$ has line of nodes at the Fermi surface. Moreover, the time-reversal symmetry is broken for $d_{x^2-y^2} + id_{xy}$-wave state.

For the pure trigonal symmetry of the CoO$_2$-plane, all three $d$-wave states are degenerate. However, due to the absence of nodes $d_{x^2-y^2} + id_{xy}$-wave seems to be most energetically favorable. Until now, a breaking of time-reversal symmetry has not been observed in experiment. Generally, the combined influence of the impurities and some competing instabilities, such as Cooper-pairing in a secondary channel as well as the lattice symmetry breaking, can lift the degeneracy be-
between these three $d$-wave competing ground states. This may indeed be the case for sodium cobaltates where Na arrangement introduces disorder at $x = 0.33$ concentration. More sophisticated theories, involving multi-orbital model for sodium cobaltates, suggest two different gap symmetries (one of which is $d_{x^2−y^2}$) for two different Fermi surface topologies.

Obviously, there is still a controversy on the symmetry of the superconducting order parameter in sodium cobaltates. In present study we systematically analyze the influence of the superconducting (SC) gap symmetry and the electronic structure on the dynamical spin susceptibility in Na$_x$CoO$_2$·H$_2$O. In particular, assuming spin singlet $s$-wave and $d$-wave symmetries of the superconducting order parameter we have calculated the real and the imaginary part of the magnetic response as a function of the momentum, temperature and frequency. We deduce the characteristic temperature dependences of the Knight shift and spin-lattice relaxation rate. Furthermore, we have studied the feedback of the superconducting order parameter on the frequency dependence of the imaginary part of the spin susceptibility. We investigate the role played by the details of the electronic structure and the energy splitting between $d_{x^2−y^2}$ hole pockets of mostly Co ions in the quasi-two-dimensional structure with Co ions in the partially filled Co-$t$-$d$ orbitals. Apart from doping, Na arrangement introduces disorder at the Co site $i$ with spin $\sigma$. Here, $\varepsilon_\mathbf{k} =$ $2t[\cos k_y + \cos (k_x\sqrt{3}/2) \cos (k_y/2)] − \mu$, $t = 0.123$ eV is the nearest-neighbor hopping integral, and $\mu$ is the chemical potential which has been calculated self-consistently for $x = 0.33$. The energy dispersion, $\varepsilon_\mathbf{k}$, along the principal directions of the hexagonal Brillouin zone (BZ) and the corresponding Fermi surface are shown in Fig. 2(b) and in Fig. 3 respectively. Here, $\Gamma = (0,0)$, $K = (0,2/3)$, and $M = (1/2\sqrt{3}, 1/2)$ [in units of $2\pi/a$] denote the symmetry points of the first BZ. Later, coordinates of the wave vectors will be given in units of $2\pi/a$ with $a$ being the in-plane lattice constant.

To calculate the dynamical spin susceptibility, we employ the Random Phase Approximation (RPA) which gives

$$\chi_{RPA}(\mathbf{q}, i\omega_n) = \frac{\chi(\mathbf{q}, i\omega_n)}{1 - \chi(\mathbf{q}, i\omega_m)},$$

where $\chi_{RPA}(\mathbf{q}, i\omega_n)$ is the BCS Lindhard susceptibility

$$\chi(\mathbf{q}, i\omega_n) = \frac{1}{2N} \sum_{\mathbf{k}} \left[ \frac{f(E_{\mathbf{k}+\mathbf{q}}) - f(E_{\mathbf{k}})}{i\omega_n - E_{\mathbf{k}+\mathbf{q}} + E_k} C_{\mathbf{k},\mathbf{q}}^+ 
+ \frac{1 - f(E_{\mathbf{k}+\mathbf{q}}) - f(E_{\mathbf{k}})}{2} C_{\mathbf{k},\mathbf{q}}^{-}
\right],$$

with $C_{\mathbf{k},\mathbf{q}} = 1 + \frac{\varepsilon_{\mathbf{k}+\mathbf{q}} + \text{Re}(\Delta_{\mathbf{k}+\mathbf{q}})}{E_k E_{\mathbf{k}+\mathbf{q}}}$ being the BCS coherence factors. Here, $\omega_n$ are the Matsubara frequencies, $f(E)$ is the Fermi function, and $E_k = \sqrt{\varepsilon_\mathbf{k}^2 + |\Delta_{\mathbf{k}}|^2}$.

In Fig. 1(a) we show both the bare and the RPA magnetic susceptibility in the normal state at $\omega = 5$ meV and $U = 0.25$ eV. One immediately notices that the magnetic response is dominated by the scattering at the incommensurate wave vector, $Q_{SDW} = (0, 0.598) \approx (0, 3/5)$. The value of Im[\chi(\mathbf{q}, \omega)] at the incommensurate wave vector, $Q_{AFM} = \{0, 2/3, 1/\sqrt{3}, 1/3\}$, appears to be much smaller. There is also another incommensurate wave vector present, $Q_{SDW}$. The presence of a set of incommensurate wave vectors with substantial magnitude of magnetic scattering shows a tendency of the itinerant electrons on the triangular lattice towards spin density wave (SDW) instability.

II. $a_{1g}$-BAND MODEL

We first consider the simple $a_{1g}$-band model, represented by a two-dimensional Hubbard Hamiltonian on the triangular lattice:

$$H = -\sum_{\mathbf{k},\sigma} \varepsilon_\mathbf{k} a^\dagger_{\mathbf{k}\sigma} a_{\mathbf{k}\sigma} + \sum_i U n_{i\uparrow} n_{i\downarrow},$$

where $n_{i\sigma} = a^\dagger_{i\sigma} a_{i\sigma}$, $a_{i\sigma}$ ($a^\dagger_{i\sigma}$) is the annihilation (creation) operator for the $a_{1g}$ hole at the Co site $i$ with spin $\sigma$. Here, $\varepsilon_\mathbf{k} =$ $2t[\cos k_y + \cos (k_x\sqrt{3}/2) \cos (k_y/2)] − \mu$, $t = 0.123$ eV is the nearest-neighbor hopping integral, and $\mu$ is the chemical potential which has been calculated self-consistently for $x = 0.33$. The energy dispersion, $\varepsilon_\mathbf{k}$, along the principal directions of the hexagonal Brillouin zone (BZ) and the corresponding Fermi surface are shown in Fig. 2(b) and in Fig. 3 respectively. Here, $\Gamma = (0,0)$, $K = (0,2/3)$, and $M = (1/2\sqrt{3}, 1/2)$ [in units of $2\pi/a$] denote the symmetry points of the first BZ. Later, coordinates of the wave vectors will be given in units of $2\pi/a$ with $a$ being the in-plane lattice constant.

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\right],$$

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becomes gapped. The magnitude of the gap, $\Omega_g$, is equal to $2\Delta_0$ in the $s$-wave case. At larger frequencies $\text{Im}\chi(0)$ increases slowly from zero. In comparison, for the $d$-wave symmetries the lowest value of $\Omega_g = |\Delta_k| + |\Delta_{k+Q}|$ at the Fermi surface. Obviously for the non-$s$-wave symme-

try it is smaller than $2\Delta_0$. From Fig. 2(a) and (b) one can notice that the $Q_{AFM}$ wave vector connects parts of the FS where $\Delta_k = -\Delta_{k+Q_{AFM}}$ but also some parts where $\Delta_k = +\Delta_{k+Q_{AFM}}$. For $d_{2z^2-r^2}$-wave superconducting gap, there are four pairs of points of the first type and two pairs of points of the second type. Due to the smaller $|\Delta_k| + |\Delta_{k+Q_{AFM}}|$ for the first process, as it is seen from Fig. 2(a), the $\text{Im}\chi(0)$ shows a discontinuous jump at $\Omega_g$. This is due to the change of sign in the anomalous coherence factor, $C_{k,q}$. The second process will give contribution at energies larger than $\Omega_g$ due to larger value of $|\Delta_k| + |\Delta_{k+Q_{AFM}}|$ there. Therefore, the net effect will result in a discontinuous jump of $\text{Im}\chi(0)$ at $\Omega_g$. Correspondingly, the real part will possess a logarithmic singularity as it is also seen in Fig. 2(d). Within the RPA the formation of the pole (spin resonance) in the total magnetic susceptibility below $\Omega_g$ is possible if $\text{Im}\chi(0) = 0$ and simultaneously $1/U = \text{Re}\chi(0)$. Due to the logarithmic character of the singularity this condition will be generally fulfilled for any small value of $U$ which would give a position of the resonance exactly at or very close to $\Omega_g$. However, a small amount of impurities or disorder will smear the singularity out and suppress the resonance peak. In Na$_2$CoO$_2$$\cdot$H$_2$O the value of $U$ should be relatively large to shift the position of the spin resonance towards energies smaller than $\Omega_g$ and make it robust against impurity scattering. The calculated susceptibility is shown in Fig. 1(c) where we use $U_{res}=0.579$ eV. It is interesting to note that the resonance occurs for both $d_{2z^2-r^2}$- and $d_{2z^2-r^2} + id_{xy}$-wave symmetries, however, the value of $\Omega_g$ slightly differs. Note, for $d_{xy}$-wave superconducting gap the situation is opposite. From Fig. 1(b) one sees that in contrast to $d_{2z^2-r^2}$-wave case there are two pairs of points at the FS where $\Delta_k = -\Delta_{k+Q_{AFM}}$ and four pairs of points where $\Delta_k = +\Delta_{k+Q_{AFM}}$. Here,
the $\Omega_g$ is determined by the second process, thus there will be no logarithmic jump in $\text{Re} \chi_0$ at $\Omega_g$. Of course it will occur at larger frequencies due to the first type of process but the resonance conditions will not be fulfilled. Therefore, we do not expect the spin resonance for the $d_{xz}$-wave symmetry.

The present value of $U_{\text{HCO}}$ is of course too small to be the on-site Coulomb repulsion which is of the order of several electron volts. Therefore, the effective interaction $U$ entering our model (1) originates mainly from the Hund’s exchange, $J_H$. In the lamellar sodium cobaltate, the value of $J_H$ is presently disputed and the lowest estimated value is of the order of 1eV. It has been shown recently that even this value significantly affects the population of the $a_{1g}$ and $e_g'$ orbitals. Taking this value into account, we assume $U = \alpha J_H$, where $J_H$ is the mean-field value of the Hund’s exchange and $\alpha$ is the coefficient that describes corrections beyond mean-field theory. One has to note that the larger value of $U$ will lead to the SDW instability in our calculations.

The situation changes for the wave vector $Q_{\text{SDW}}$ [Fig. (1f)-(h)]. There is one striking difference in the low-energy behavior of $\text{Im} \chi_{Q_{\text{SDW}}, \omega}$. Namely, already in the normal state the scattering rate is non-linear for small $\omega$. It is obviously a consequence of the $2k_F$ instability and a resulting non-Landau damping at this wave vector. Furthermore, in the SC state the situation differs drastically with respect to $Q_{\text{AFM}}$. As one could see from Fig. (2c) and (d) there is equal number of contributions for which $\Delta_k = -\Delta_{k+Q_{\text{SDW}}}$ and $\Delta_k = +\Delta_{k+Q_{\text{SDW}}}$. As a result the discontinuity does not occur and the real part of $\chi_0$ is smaller in the superconducting state than in the normal state. Therefore, for reasonable values of $U$ there is no resonance condition for $\chi_{\text{RPA}}$ [see Fig. (1h)].

Generally, a formation of the resonance peak below $T_c$ in the unconventional superconductors is a well-known consequence of the sign change of the superconducting order parameter. It has been originally discussed in relation to the layered high-$T_c$ cuprates and also recently has been used to explain the inelastic neutron scattering results in heavy-fermion compound UPd$_2$Al$_3$. In layered superconducting cobaltates the emergence of the resonance peak for several symmetries of the superconducting order parameter has been analyzed within simple single-band model. In contrast to Ref. 42, we have found that the resonance peak (even within simple $a_{1g}$-band model) is very sensitive to the small variation of $U$-values and to disorder. As a result the resonance is confined to the wave vector $Q_{\text{AFM}}$ and disappears for $|Q| < |Q_{\text{AFM}}|$.

The temperature dependence of the Knight shift, $K(T)$, and the spin-lattice relaxation rate, $1/T_1T$, is calculated according to the expressions:

$$K(T) \propto \lim_{\omega \to 0} \text{Re} \chi(q, \omega), \quad (4)$$

$$1/T_1T \propto \lim_{\omega \to 0} \frac{1}{\pi} \sum_q \frac{\text{Im} \chi(q, \omega)}{\omega}. \quad (5)$$

In Fig. 3 we show both quantities as a function of temperature. In the normal state $1/T_1T$ increases with decreasing temperature that reflects the presence of the incommensurate antiferromagnetic fluctuations in this system. At the same time, the Knight shift is a constant which stresses that there are no small-$q$ fluctuations. Below $T_c$ both physical observables drop rapidly due to opening of the superconducting gap in the energy spectrum. As expected, the decrease is exponential for $d_{xz}$-wave symmetry due to its nodeless character in $E_k$. For $d_{xy}-$wave symmetry the behavior of $1/T_1T$ and $K(T)$ follows standard power-law temperature dependence due to the presence of the line nodes in the energy spectrum. In the next section we will compare our results to the experimental data where we describe a more realistic model in application to the superconducting cobaltate.

### III. $t_{2g}$-BAND MODEL

The $a_{1g}$-band model is, of course, oversimplified for describing the physics of Na$_x$CoO$_2$.yH$_2$O since $a_{1g}$-$e_g'$ level splitting, $\delta \epsilon$, is only 53 meV. As a result there is a substantial hybridization of the $a_{1g}$ and the $e_g'$ bands, completely neglected in the simple $a_{1g}$-band model. In particular, the $e_g'$ bands may form hole pockets at the FS in addition to a large $a_{1g}$-pocket. To take into account these details, we further analyze the magnetic response in the full $t_{2g}$-band model including both $a_{1g}$ and $e_g'$ cobalt states.

The free electron Hamiltonian of the $t_{2g}$-band model in a hole representation is given by

$$H_0 = - \sum_{k, \alpha, \sigma} (\epsilon_\alpha - \mu) n_{k\alpha\sigma} - \sum_{k, \sigma} \sum_{\alpha, \beta} t_{k}^{\alpha \beta} d_{k\alpha\sigma}^\dagger d_{k\beta\sigma}, \quad (6)$$

where $n_{k\alpha\sigma} = d_{k\alpha\sigma}^\dagger d_{k\alpha\sigma}$, $d_{k\alpha\sigma}$ ($d_{k\alpha\sigma}^\dagger$) is the annihilation (creation) operator for the $t_{2g}$-hole with spin $\sigma$, orbital index $\alpha$, and momentum $k$, $t_{k}^{\alpha \beta}$ is the hopping matrix element, $\epsilon_\alpha$ is the single-electron energy, and $\mu$ is the chemical potential. All of the in-plane hoppings and
the single-electron energies were derived previously by us from the \textit{ab-initio} LDA calculations using projection procedure and we use here the parameters for $x=0.33$ from Ref. 35. To obtain the dispersion we diagonalize the Hamiltonian \cite{28} calculating the chemical potential $\mu$ self-consistently. The resulting FS topology and energy dispersion are shown in Fig. 4(b) and (c), respectively. The resulting dispersion and the FS replicate the corresponding LDA ones\cite{28}.

Due to the non-zero inter-orbital hopping matrix elements, $a_{1g}$ and $c'_{g}$ bands are hybridized. However, only one of the hybridized bands crosses the Fermi level thus making the largest contribution to the low-energy properties of the system. We refer to this band as $\varepsilon_1$. Note, it is substantially different from the simple $a_{1g}$-band. Later, this effective band $\varepsilon_1$ will be used to calculate the dynamical magnetic susceptibility with some effective onsite Coulomb interaction $U$.

Present FS has more complicated structure in comparison to the $a_{1g}$-band model. First, $e'_{g}$ states are present at the Fermi surface and strongly hybridize with $a_{1g}$ states. At the same time, the “rounded hexagon” shape of the central part of the FS arises from the hoppings beyond nearest-neighbors included in the $t_{2g}$-band model and neglected in $a_{1g}$-band model considered above. This results in a number of additional scattering wave vectors as calculated from $\chi_0$, see Fig. 4(a). In particular, there are four scattering wave vectors connecting the $e'_{g}$ band $\varepsilon_1$ FS pockets $Q_{e'}$, $Q_{e''}$, $Q_{e'''}$, and $Q_{SDW_2} = (0, 0.495)$, and also two scattering wave vectors connecting the $a_{1g}-c'_{g}$ FS pockets $Q_{e'}$ and $Q_{SDW_1}$. At the same time, these wave vectors also connect parts of the central $a_{1g}$ FS pocket and the total magnetic susceptibility includes contribution from this scattering too. In addition, there are two wave vectors, $[Q_{AFM}$ and $Q_{SDW_1} = (0, 0.649)]$ which arise due to the curved form of the central $a_{1g}$ FS pocket. The pronounced peaks at all these wave vectors are present in both the bare and the RPA magnetic susceptibility ($U=0.15$ eV). Again, similar to the $a_{1g}$-band model, the magnetic response is not dominated by the scattering at the commensurate wave vector $Q_{AFM}$. The overall picture of the magnetic response is consistent with the one presented in Ref. 15.

In the non-SC phase and the SC phase with $s$-wave order parameter the behavior of $\chi(q, \omega)$ at $q = Q_{AFM}$ \cite{28} is similar to the one in the $a_{1g}$-band model. However, for the $d$-wave symmetry of the order parameter, one finds that for $\omega \geq \Omega_g$ the states with equal signs of the superconducting order parameter \cite{29} contributes first, and the discontinuous jump in Im$[\chi_0(Q_{AFM}, \omega)]$ occurs at higher energies. The particular form of the FS in the realis-
tactic $t_{2g}$-band model and more complicated band structure produce this effect. Therefore, the resonance peak in $\text{Im}[\chi_{RPA}(Q_{\text{AFM}}, \omega)]$ may in principle still exist, however, it occurs in a very narrow interval of the $U$ values. This interval is determined by the resonance condition in the superconducting state and by the stability of a para-magnetic state above $T_c$. Here, we use $U_{\text{res}} = 0.26$ eV, which is more than twice smaller than in the $a_{1g}$-band model.

Although the formation of the spin resonance is unrealistic for the antiferromagnetic wave vector $Q_{\text{AFM}}$ it may now occur at other wave vectors. In Fig. 4(g)-(j) we present the imaginary parts of $\chi_{\text{AFM}}$ and $\chi_{RPA}$ at $Q_{\text{SDW}}$ and at $Q_{\text{SDW2}}$. Here, one notices the pronounced effects of the complicated $t_{2g}$-band structure at high energies for the scattering at both wave vectors. Deviations from the linear-$\omega$ damping start already at low energies, smaller than $\Omega_g$. For $U = U_{\text{res}}$ the spin-resonance is present at $Q_{\text{SDW}}$ for both $d$-wave symmetries. However, at $Q_{\text{SDW2}}$ the resonance peak is present for $d_{x^2-y^2} + id_{xy}$-wave symmetry only. Similar to the situation with $Q_{\text{AFM}}$, this is due to smallness of the allowed $U$ values.

In Fig. 5 we show the corresponding results for the $1/T_1(T)$ and $K(T)$. Below superconducting transition temperature the behavior is very similar to the results obtained for the simple $a_{1g}$-band model. This is because below $T_c$ the symmetry of the superconducting gap and its nodal structure determines the temperature dependencies of the $1/T_1(T)$ and the $K(T)$ values. At the same time, notice the stronger AFM fluctuations in the normal state. For almost the same value of $U$ as in Fig. 4 this is due to the larger density of states at the Fermi level (and the change of the Fermi velocity) than in the simple $a_{1g}$-band model. Such a behavior is observed in the experimental NQR data. It is interesting to note that without water the parent non-superconducting compound Na$_{0.3}$CoO$_2$ shows much weaker AFM fluctuations. In our theory the fluctuations occur for the parent compound too. It probably demonstrates a significant difference with the third dimension and in particular, the bilayer splitting which may reduce the two-dimensional AFM fluctuations in Na$_{0.3}$CoO$_2$.

Note, the presence of the $e'_g$ pockets on the FS can also lift the degeneracy between the three $d$-wave states. Since in the $d_{x^2-y^2}$-wave SC state the $e'_g$ FS pockets are fully gapped, the additional condensation energy is gained [compare the topology of the line-nodes in Fig. 2(a) and FS topology in Fig. 4(b)]. For the $d_{xy}$-wave SC state this gain in energy will be smaller [compare Fig. 2(b) and FS in Fig. 4(b)].

Presently, there is still a discussion on the details of the Fermi surface topology in the water intercalated cobaltates. In particular, ARPES experiments do not observe the $e'_g$ pockets at the FS. It has been shown that an inclusion of the electronic correlation within Gutzwiller approximation may shift the $e'_g$-bands below the Fermi level, although this conclusion has been challenged. Another interpretation of this experimental result relies on the disorder introduced by Na. As it was shown within LDA, the scattering due to disorder can destroy the small $e'_g$-pockets. For the superconducting polycrystalline samples, recent experiments indicate that the oxonium ions, H$_3$O$^+$, may introduce additional dopants, or result in oxygen vacancies reducing Co oxidation state. Though, this conclusion
has been doubted by the NMR experiments which show the Co valence state is insensitive to hydration and depends on the Na content only. This was also confirmed later by the powder neutron diffraction.

In our study we further consider the $t_{2g}$-band model with increased crystal field splitting, $\delta e=153$ meV. This makes $e'_g$ band sink below the Fermi level, as it is seen in the inset of Fig. 6(a). The behavior of the dynamical spin susceptibility for $U=0.15$ eV at $\omega = 5$ meV presented in Fig. 6(a) shows more similarity to the simple $a_{1g}$-band model with additional features due to peculiarities (“rounded hexagon” form) of the large FS pocket as shown in Fig. 6(b). The scattering is most pronounced at the wave vector $Q_{SDW} = (0,0.633)$. There is also intensive scattering at the wave vector $Q_{SDW}^g$, owing its appearance to the curved shape of the FS.

Fig. 6(c)-(e) and (f)-(h) displays the magnetic susceptibility at $Q_{AFM}$ and at $Q_{SDW}$, respectively. Contrary to both $a_{1g}$-band model and $t_{2g}$-band model with $e'_g$ FS pockets, here we observe a well-defined linear behavior of $\text{Im}[\chi_0(q,\omega)]$ in the considered frequency range at these wave vectors. For the $d$-wave order parameter, the behavior of the susceptibility resembles that in the $t_{2g}$-band model with $e'_g$ FS pockets. Again one could find a narrow range of parameters where the resonance peak exists, which we illustrate in Fig. 6(e),(h) for $U_{res}=0.342$ eV.

Similarly, the change of the FS topology does not influence significantly the temperature dependence of the Knight shift and the spin-lattice relaxation rate above and below $T_c$. This is illustrated in Fig. 7 where we plot both quantities as a function of temperature.

IV. CONCLUSION

Our analysis of the dynamical spin susceptibility in application to the $\mathrm{Na}_x\mathrm{CoO}_2\cdot y\mathrm{H}_2\mathrm{O}$ have shown that the magnetic response in the normal state is dominated by the incommensurate SDW fluctuations at large momenta close to $Q_{AFM}$. This is consistent with experimental NQR data which shows a pronounced AFM-like fluctuations in the temperature dependence of the spin-lattice relaxation rate. It is interesting to note that the presence of the $e'_g$-pockets at the Fermi surface is not affecting significantly this result. In the normal state we note the absence of ferromagnetic-like fluctuations. This observation justifies our choice of spin-singlet order parameter, because to induce the spin-triplet Cooper-pairing the fluctuations with small momenta are required. Below $T_c$ our results for $d_{x^2-y^2}$ or $d_{xy}$-wave (not shown) symmetries of the superconducting order parameter are consistent with experimental data which excludes nodeless $d_{x^2-y^2}$ or $id_{xy}$-wave symmetry. We further stress that the resonance peak, predicted previously for the simple $a_{1g}$-band model, is improbable for the realistic band structure of $\mathrm{Na}_x\mathrm{CoO}_2\cdot y\mathrm{H}_2\mathrm{O}$. Moreover, we find that even if present the resonance peak is confined to the AFM wave vector and disappears away from it.

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