Quantum Ising model coupled with conducting electrons

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Abstract. The effect of photo-doping on the quantum paraelectric SrTiO$_3$ is studied by using the one-dimensional quantum Ising model, where the Ising spin describes the effective lattice polarization of an optical phonon. Two types of electron-phonon couplings are introduced through the modulation of transfer integral via lattice deformations. After the exact diagonalization and the perturbation studies, we find that photo-induced low-density carriers can drastically alter quantum fluctuations when the system locates near the quantum critical point between the quantum para- and ferroelectric phases.

1. Introduction
The static dielectric permittivities of the quantum paraelectric (QPE) perovskites, such as SrTiO$_3$ (STO) and KTaO$_3$, first follow the Curie-Weiss law at high temperatures, but with decreasing temperature it does not show any diverging behavior in contrast to the usual paraelectrics or ferroelectrics. Instead, the QPE dielectric permittivity increases monotonically to crossover into temperature-independent at the lowest temperature. This temperature profile can be roughly fitted to the Barrett formula, which is an extension of the “Slater’s Curie-Weiss law for the ferroelectric BaTiO$_3$” to include the zero-point fluctuation of phonons. In the QPE ground state, not thermal fluctuations but quantum fluctuations destabilize the ferroelectric long-range order at zero temperature. This statement clearly indicates the fact that the quantum nature of phonons is indispensable in the physics of QPE. The proximity to the QPE/ferroelectric (FE) quantum critical point makes QPE materials more attractive because highly enhanced fluctuations sometimes induce collective phenomena. From the experimental point of view, it has been found in SrTiO$_3$ that small external perturbations, such as an electric field, uniaxial pressure, cation (Ca$^{2+}$) doping, and isotope ($^{18}$O) substitution, suppress quantum fluctuations to realize the ferroelectric ground state beyond the critical point.

The recent experiments with ultraviolet light irradiation to the QPE SrTiO$_3$ elucidate that i) an incident light furthermore enhances the low-temperature dielectric permittivity and ii) the photoinduced carriers identified as electrons by the photo-Hall measurement have rather high mobility[1, 2, 3]. Fluctuations of polar phonon modes and the photoinduced electrons are expected to play major roles in this phenomenon because the above experimental results are observed only in the QPE STO, but not in the FE $^{18}$O-substituted SrTi$^{18}$O$_3$, and only when the energy of the incident light ($h\nu \sim 3.8$ eV) exceeds the band gap ($\sim 3.2$ eV) of STO.

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The band-structure calculation of STO shows that the width of the conduction band, which mainly consists of Ti-$t_{2g}$ orbitals, is about 1 eV corresponding to an electron transfer integral $t$ of the order of 1000 K\cite{4}. On the other hand, the best fit to the Barrett formula of the observed dielectric permittivity in STO gives $T_1 \sim 72$ K and $T_0 \sim 32$ K, where $T_1$ represents the magnitude of quantum fluctuations and $T_0$ corresponds to the classical Curie temperature. Since the characteristic energy scale of electrons ($t$) is much higher than that of phonons ($T_1$ or $T_0$), an optimized electronic configuration would result in significant redistribution of phonons. It is not surprising that the injected electrons contribute to dielectric fluctuations through an electron-phonon coupling. However the effective mass of phonon-dressed electrons is generally expected to be heavy. Therefore, it is important to explain both the enhancement of permittivity and the high mobility (light effective mass) simultaneously.

2. Model Hamiltonian

Let us start from the quantum Ising model which was originally introduced into this field to describe the “order-disorder type” ferroelectric transition,

$$H_{\text{QI}} = h \sum_i \sigma_i^z - J \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z,$$

(1)

where the lattice deformation accompanying an electric dipole moment is described by a pseudospin with the Pauli matrix $\vec{\sigma}_i$. Within the mean field approximation, the dielectric susceptibility of the quantum Ising model is given by the Barrett formula in the form;

$$\varepsilon(T, h, J) = \frac{1}{h \coth \frac{h}{T} - zJ},$$

(2)

where $z$ is the coordination number. For $h > zJ$, $\varepsilon(T)$ increases toward $1/(h - zJ)$ as $T \to 0$ and the QPE ground state is realized. In contrast, for $h < zJ$, $\varepsilon(T)$ diverges at a finite temperature where the usual PE-to-FE phase transition takes place. In comparison with the original Barrett formula, the relations $h = T_1/2$ and $zJ = T_0$ hold. The usage of $H_{\text{QI}}$ is justified by the fact that the electric-field-dependent dielectric permittivity in STO is almost perfectly explained by the mean-field analysis of $H_{\text{QI}}$ under the uniform electric field of $-EF\sum_i \sigma_i^z$\cite{5}. This quantum Ising model is also applied to explain the recently found O-substitution induced QPE/FE phase transition in SrTiO$_3$\cite{6}. Thus in order to study the photodoping effects near the QPE/FE critical point, we employ the simple one-dimensional quantum Ising model coupled to low-density electrons. The electronic part of the Hamiltonian is assumed to be of the spinless tight-binding model, $H_d = -t \sum_i (d_i^\dagger d_{i+1} + d_{i+1}^\dagger d_i)$, and the Coulomb interaction is ignored since we only think about the low-carrier limit. In one dimension, $H_{\text{QI}}$ is integrable by applying the Jordan-Wigner transformation. The exact result shows that strong fluctuations modify the above mentioned critical point $(h/J)_c$ from $z$ to unity.

In general, electron transfers between neighboring titanium sites are modulated by lattice displacements. We take the lowest-order modulations as effective electron-phonon interactions which are represented by couplings between the pseudospin and the electron. In SrTiO$_3$ the bare hopping integral $t$ in $H_d$ is about 1000 K as mentioned above, while the parameters in the quantum Ising model $h$ and $J$ are estimated to be 36 K and 32 K, respectively. To be explicit, we have introduced two different kinds of hopping modulations as follows;

$$H_\alpha = \alpha \sum_{i=1}^N (\sigma_{i+1}^z - \sigma_i^z)(d_{i+1}^\dagger d_i + d_i^\dagger d_{i+1}) = \frac{1}{N} \sum_{kq} i\alpha_{kq} \sigma_k^z \cdot d_{k+q}^\dagger d_k,$$

(3)

$$H_\beta = \beta \sum_{i=1}^N (\sigma_{i+1}^z - \sigma_i^z)^2 (d_{i+1}^\dagger d_i + d_i^\dagger d_{i+1}) = \beta \sum_{i=1}^N (2 - 2\sigma_{i+1}^z \sigma_i^z)(d_{i+1}^\dagger d_i + d_i^\dagger d_{i+1}),$$

(4)
where $\alpha_{kq} = 4\alpha \cos \left( k + \frac{q}{2} \right) \sin \frac{q}{2}$. In the $\alpha$ and $\beta$ terms, the local dielectric moment at each site is aligned parallel and perpendicular to the chain direction, respectively, as shown in figure 1. The signs of both $\alpha$ and $\beta$ are reasonably assumed to be positive by evaluating the overlap of wavefunctions. Since the definition of $\vec{\sigma}_i$ is different in Eqs. (3) and (4), the $\vec{\sigma}_i$ operators in $H_{QI}$ should be read correspondingly depending on the model considered; $H_{QI} + H_{\alpha}$ or $H_{QI} + H_{\beta}$.

**Figure 1.** The directions of local dipole moments ($\sigma_i$) for the $\alpha$ and $\beta$ terms.

3. Results and discussions

To see how the electron-phonon coupling terms (3) and (4) control the QPE/FE quantum critical point, we perform the numerical exact diagonalizations on $H_d + H_{QI} + H_{\alpha}$ and $H_d + H_{QI} + H_{\beta}$. The system size used is 12 sites with a single electron. In the numerical calculations $t$ is always fixed to $30J$ and $h$ varies from 0 to $2J$, where $h = 1.2J$ corresponds to the experimental parameter for STO. Without $\alpha$ or $\beta$, the excitation gap $\Delta$ is proved to vanish at the quantum critical point as $\Delta/J = 2|h/J - 1|$. Numerically, this critical point can be estimated from the linear extrapolation of the calculated energy gap away from the critical point, to avoid the finite size effect that dominates over the critical point. The shift of the critical point after including $\alpha$ or $\beta$ has been estimated in the same way (figure 2). The results are summarized as follows. In the case of $\alpha > 0$ the FE region is suppressed and $(h/J)_c$ decreases from unity as a quadratic function of $\alpha$. In contrast, for $\beta > 0$ the FE region is extended and $(h/J)_c$ increases as a linear function of $\beta$. The energy scale of $\beta$ is about an order of magnitude smaller than that of $\alpha$ to give the same (absolute) amount of the critical point shift.

Since $H_{\alpha}$ or $H_{\beta}$ term has a much smaller energy scale than the tight-bind Hamiltonian $H_d$, we can perturbatively derive the effective pseudospin Hamiltonian after integrating out the electron degrees of freedom. For the $\alpha$ term the lowest order perturbation gives that

$$H_{\alpha}^{(2)} = -\frac{1}{N} \sum_q \chi_q \sigma_q^z \sigma_{-q}^z \text{ with } \chi_q = \frac{1}{N} \sum_{|k| \leq k_F} \frac{\alpha_{kq}^2}{\varepsilon_k - \varepsilon_{k+q}} \propto \frac{e^2}{t} k_F. \quad (5)$$

In the $H_{QI} + H_{\alpha}^{(2)}$ model, the anomaly of $\chi_q$ at $q = 2k_F$ will enhance the dielectric fluctuations at $q = 2k_F$ but reduces those at $q = 0$. The energy shift due to $H_{\alpha}^{(2)}$ is proportional to $\alpha^2/t$, which is consistent with the numerical results. In the case of the $\beta$ term,

$$H_{\beta}^{(1)} = -\sum_i \tilde{\varepsilon}_0 \sigma_i^z \sigma_{i+1}^z \text{ with } \tilde{\varepsilon}_0 = \frac{4}{N} \sum_{|k| \leq k_F} \beta k \cos k \propto \beta k_F. \quad (6)$$

This effective Hamiltonian only changes $J$ in $H_{QI}$ into $J + \tilde{\varepsilon}_0$, which is advantageous to the FE state because $\tilde{\varepsilon}_0 > 0$. The $\beta$-linear dependence of $\tilde{\varepsilon}_0$ is also in accordance with the numerical results.

Next we estimate the effective mass $m^*$ by calculating the quantity $\langle d^\dagger_{i+1} d_i + d^\dagger_i d_{i+1} \rangle \propto 1/m$. Figure 3 shows the effective mass as a function of $\alpha$ or $\beta$ for a fixed value of $h/J = 1.2$. It is
clear that $m^*$ is largely enhanced by the $\alpha$ term when compared with the enhancement by the $\beta$ term. The origin of this difference can be explained by calculating correlation functions as schematically shown in figure 4. In the case of the $\alpha$ term the phase of the lattice displacement is changed by $\pi$ around an electron and the dielectric permittivity drops. Namely, when an electron moves by one site, the overlap with the original configuration is small, which means that the effective transfer between neighboring sites is reduced. In the case of the $\beta$ term, however, electrons align the surrounding pseudo spins parallel to each other, the permittivity is enhanced, and the effective electron transfer does not change sizably. This appears consistent with the experimental results. The light effective mass of electrons coupled with phonons is obtained in a different model also[7].

Figure 3. The effective mass enhancement as a function of $\alpha$ (left) and $\beta$ (right) for the fixed value of $h/J = 1.2$

4. Summary
In order to explain the enhanced static dielectric permittivity and the large mobility observed in the photo-carrier doped STO, we examined the effects of electron-phonon interactions near
Figure 4. Snapshots of the lattice displacement around a single electron located on the filled circle for the $\alpha$ (left) and $\beta$ (right) terms.

the QPE/FE quantum critical point. A photocurrent perpendicular to the local electric dipole moment enhances the dielectric fluctuation without changing the effective mass of electrons sizably.

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References
[1] Takesada M, Yagi T, Itoh M, and Koshihara S 2003 J. Phys. Soc. Jpn. 72 37
[2] Hasegawa T, Mouri S, Yamada Y, and Tanaka K 2003 J. Phys. Soc. Jpn. 72 41
[3] Ishikawa T, Kurita M, Shimoda H, Sakano Y, Koshihara S, Itoh M, and Takesada M 2004 J. Phys. Soc. Jpn. 72 1635
[4] Uchida K and Tsuneyuki S 2003 Phys. Rev. B 68 174107
[5] Hemberger J, Lunkenheimer P, Viana R, Böhmer R, and Loidl A 1995 Phys. Rev. B 52 13159
[6] Yamada Y, Todoroki N, and Miyashita S 2004 Phys. Rev. B 69 024103
[7] Nasu K 2003 Phys. Rev. B 67 174111