

## Effect of electron correlation on vibrational frequencies of $A_g$ modes in $C_{60}$

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The effect of electron correlation on the vibrational frequencies of two  $A_g$  modes in  $C_{60}$  is studied by using the Gutzwiller ansatz to construct the correlated wave function. It is found that the electron correlation decreases the frequencies of the  $A_g$  modes if the electron-phonon coupling is weak, whereas the correlation increases these frequencies if the electron-phonon coupling is strong. For the realistic strength of the electron-phonon and electron-electron interactions in  $C_{60}$ , the correlation results in an observable reduction of the frequencies of these modes. The physical reasons of these features are discussed.

### I. INTRODUCTION

The superconductivity found in the alkali-metal-doped  $C_{60}$  system<sup>1</sup> has stimulated studies of its mechanism.<sup>2-4</sup> It is still a controversial subject whether the superconductivity is due to the conventional electron-phonon ( $e-p$ ) interaction or to the electron-electron ( $e-e$ ) correlations. Nevertheless, the  $^{13}\text{C}$  isotope effect of  $T_c$ <sup>5-8</sup> supports the idea that there are large phonon contributions to the mechanism of superconductivity. In solid  $C_{60}$ , since the molecules are linked by the weak van der Waals interaction, and the electron-intramolecular-vibration coupling is predominant over the electron-intermolecular-vibration coupling, so, a study of the vibrations of a single  $C_{60}$  molecule should be helpful to understand the role of phonons in the superconductivity. Several efforts have been undertaken to study the vibration in  $C_{60}$ , e.g., Weeks and Harter<sup>9</sup> gave an elegant icosahedral analysis to determine the normal modes and their frequencies of a classical spring mass model of  $C_{60}$ , and You *et al.*<sup>10</sup> applied the tight-binding Su-Schrieffer-Heeger-like Hamiltonian, which was originally introduced to demonstrate the presence of the soliton in polymer,<sup>11</sup> and studied the effect of  $e-p$  coupling on the vibration of  $C_{60}$ .

But there is evidence that the  $e-e$  interaction is important to determine the properties of  $C_{60}$ , and many theoretical calculations and experiments indicate that the molecule  $C_{60}$  is a strong-correlated system with the presence of a moderate bare on-site Coulomb interaction ( $U \sim 6-12$  eV).<sup>12-14</sup> To illustrate the electron correlation, the Hubbard model on a single  $C_{60}$  has been previously discussed by Chakravarty, Gelfand, and Kivelson<sup>12</sup> in the weak-coupling regime and Sheng *et al.*<sup>15</sup> in large-

$U$  version or equivalently the  $t$ - $J$  model. They used perturbation theory and variational Monte Carlo method to investigate the ground state of doped and undoped  $C_{60}$ . However, understanding of the influence of the Hubbard repulsion on vibrational properties in  $C_{60}$  has not yet been fully established. Salkola *et al.* added a Hubbard term in the Su-Schrieffer-Heeger-like Hamiltonian and discussed this issue, but their treatment of the  $e-e$  correlation is only at a second perturbation level and includes some additional approximations.<sup>16</sup> To clarify the correlation effect on the vibration in  $C_{60}$ , in this paper, we will go beyond perturbation theory to study the same model of Ref. 16.

Since the realistic strength of  $e-e$  interaction in  $C_{60}$  is in the intermediate-coupling regime, neither weak nor strong coupling, both a perturbation theory and a large- $U$  approximation do not work. To make our calculation more convincing, we will use the Gutzwiller variational ansatz<sup>17</sup> to construct the ground-state wave function, which is very analogous to that developed by Horsh<sup>18</sup> and Baeriswyl and Maki<sup>19</sup> in polyacetylene. This approach is valid in the region ranging from weak to intermediate coupling. Actually, we have already applied it to investigate the correlation effect on the bond structure in  $C_{60}$ ,<sup>20</sup> and found that the length difference between the long and short bonds is enhanced considerably by the correlation within the realistic strength of the Hubbard interaction. Among the numerous kinds of vibrational modes in the  $C_{60}$ , two full-symmetric  $A_g$  modes are very important and interesting. In the Raman spectra, these modes are much more intense than other modes,<sup>21</sup> moreover, they preserve the icosahedral symmetry and the bond-bending effect has no contribution, so the adjustable

parameters are fewer and this makes it easier to study the correlation effect on the vibration in  $C_{60}$ . From the influence of  $e$ - $e$  correlation on these two modes, we can estimate the correlation effect on other modes. In this paper, we will focus on these two full-symmetric  $A_g$  modes and study the correlation effect on their frequencies. In Sec. II, the Hamiltonian is defined and the formulations are worked out. In Sec. III, we present numerical results as well as the physical analysis.

## II. FORMALISM

The  $\pi$ -electron tight-binding model of the molecule  $C_{60}$  reads<sup>20</sup>

$$H = H_0 + H_{\text{int}}, \quad (1)$$

$$H_0 = - \sum_{\langle ij \rangle \sigma} h_{ij} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.}), \quad (2)$$

$$H_{\text{int}} = U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (3)$$

$c_{i\sigma}^\dagger$  ( $c_{i\sigma}$ ) denotes the creation (annihilation) operator of an electron with spin  $\sigma$  at site  $i$ , and  $n_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$ .  $j$  and  $i$  are nearest neighbors,  $\sum_{\langle ij \rangle}$  means summation over the bonds, and

$$h_{ij} = t_0 - \alpha(d_{ij} - d_0), \quad (4)$$

$t_0$  is the hopping constant,  $\alpha$  the electron-lattice coupling,  $d_0 = 1.54$  Å the bond length of diamond,  $d_{ij}$  the bond length between  $i$  and  $j$  atoms.

In the ground state,  $C_{60}$  possesses the structure of truncated icosahedron consisting of 20 hexagons and 12 pentagons, and in this allotrope, 60 carbon atoms are equivalent. We can construct the ground-state wave function using the Gutzwiller ansatz<sup>17-19</sup>

$$|\psi\rangle = e^S |0\rangle, \quad (5)$$

where  $|0\rangle$  is the ground state of the single-particle Hamiltonian  $H_0$ , and

$$S = -\frac{1}{2}\eta \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (6)$$

Here, a parameter  $\eta$  has been introduced to describe the effect that the Hubbard interaction prevents double occupation at one site. We have made an approximation by using a global correlation parameter instead of site-varying one, this is reasonable because of the equivalence of carbon atoms in  $C_{60}$ . In the  $C_{60}$ , there are only two different types of C-C bonds: a long bond between a pentagon and a hexagon and short bond between two hexagons. Including the elastic energy of 60 long bonds and 30 short bonds associated with the  $\sigma$ -bond compression, we can write the total energy as

$$\mathcal{E}(\eta, d_1, d_2) = \frac{60}{2}K(d_1 - d_0)^2 + \frac{30}{2}K(d_2 - d_0)^2 + \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle, \quad (7)$$

$K$  is stiffness constant of the bond-stretching spring,  $d_1$  and  $d_2$  are the lengths of the long bond and short bond, respectively.

Expanding  $e^S$  to second order in  $\eta$ , and minimizing the total energy with respect to  $\eta$  first, we obtain the expression of the energy as a function of  $d_1$  and  $d_2$ ,<sup>20</sup>

$$\mathcal{E}(d_1, d_2) = \frac{60}{2}K(d_1 - d_0)^2 + \frac{30}{2}K(d_2 - d_0)^2 + W_0 - \frac{W_1^2}{4W_2}, \quad (8)$$

where

$$W_0 = -2 \sum_{\langle ij \rangle \sigma} h_{ij} P_{ij} + 60 \frac{U}{4}; \quad (9)$$

$$W_1 = -U \sum_{lm} P_{lm}^4, \quad (10)$$

$$W_2 = - \sum_{\langle ij \rangle \sigma} h_{ij} \left[ -\frac{1}{8}P_{ij} - \frac{1}{2}P_{ij}^3 + \sum_l (P_{il}^3 P_{lj} + P_{il} P_{lj}^3) - \sum_{lm} 2P_{ml}^3 P_{li} P_{mj} \right] + \frac{1}{2}U \sum_{lmn} (Q_{lm} P_{mn} P_{nl} - P_{lm} Q_{mn} Q_{nl})^2. \quad (11)$$

The summation for  $l, m, n$  is from 1 to 60, representing 60 sites, while, the summation for  $\langle i, j \rangle$  is over 90 bonds. The correlation functions are defined as

$$P_{ij} \equiv \langle 0 | c_{i\sigma}^\dagger c_{j\sigma} | 0 \rangle \quad \text{and} \quad Q_{ij} \equiv \langle 0 | c_{i\sigma} c_{j\sigma}^\dagger | 0 \rangle = \delta_{ij} - P_{ij}.$$

Here, we have assumed that the spin symmetry in the ground state is not broken, this is reasonable for the moderate  $e$ - $e$  coupling.<sup>19</sup> The correlation functions can be calculated by

$$P_{ij} = \sum_k^{\text{occ}} \langle g_k | i \rangle \langle j | g_k \rangle, \quad (12)$$

where  $g_k$  is the eigenstate of the single-electron Hamiltonian  $H_0$  with bond-length parameters  $d_1$  and  $d_2$ . The summation for  $k$  is over all occupied single-electron states.

Minimizing the expression Eq. (8) with respect to  $d_1$  and  $d_2$ , we can obtain the long bond length  $\tilde{d}_1$  and short bond length  $\tilde{d}_2$  in the ground state. The two  $A_g$  modes of the vibration maintain the icosahedral symmetry of the  $C_{60}$  molecule. For the lower-frequency mode [named  $A_g(I)$ ], we can interpret that each atom vibrates along the radial direction with the same amount; for the higher-frequency one [named  $A_g(II)$ ], we can interpret that the long bonds are stretched an amount of  $u$ , and the short bonds are compressed an amount of  $2u$  in order not to destroy the icosahedral symmetry and keep the average length unchanged.<sup>10</sup> In the adiabatic approximation, the frequencies of these two modes are determined by the effective force constants associated with these modes. For the  $A_g(I)$  mode, the radius of the  $C_{60}$  has deviated from the equilibrium value  $r_0$  to  $r = r_0 + a \equiv r_0 \gamma$ ; if we denote  $F_1(a) = \mathcal{E}(\tilde{d}_1 \gamma, \tilde{d}_2 \gamma)$ , the effective force constant of the  $A_g(I)$  mode is obtained by

$$K_1^{\text{eff}} = \frac{1}{60} \frac{d^2 F_1}{da^2}, \quad (13a)$$

and the effective force constant of the  $A_g(II)$  mode can be written as

$$K_2^{\text{eff}} = \frac{1}{60} \frac{d^2 F_2}{du^2}, \quad (13b)$$

where  $F_2(u) = \mathcal{E}(\bar{d}_1 + u, \bar{d}_2 - 2u)$ . Thus, the frequencies of these two modes  $\bar{\omega}_i = \sqrt{K_i^{\text{eff}}/M}$  ( $i=1,2$ ),  $M$  is the mass of carbon atom.

### III. RESULTS AND DISCUSSIONS

To shed some light on the physical origin of the correlation effect, at first we calculate the frequencies of these two modes with varying  $e$ - $p$  coupling in the absence of the Hubbard interaction. It is useful to introduce the dimensionless parameter  $\lambda = 2\alpha^2/(\pi K t_0)$  to measure the strength of  $e$ - $p$  coupling.<sup>11</sup> For the realistic parameters of  $C_{60}$  used in Ref. 10,  $t_0 = 1.91$  eV,  $\alpha = 5.0$  eV/Å,  $K = 42.0$  eV/Å<sup>2</sup>, the  $e$ - $p$  coupling constant is relatively small,  $\lambda = 0.198$ . Although the real  $C_{60}$  molecule lies in the regime of the weak  $e$ - $p$  coupling, we will change the  $e$ - $p$  coupling strength in a broad range in our calculations. These calculations are helpful to reach an unified physical picture of the correlation effect in different  $e$ - $p$  coupling regions. In following discussions, we fix the value of  $K$  to ensure the unscreened phonon frequencies do not change. For  $K = 42.0$  eV/Å<sup>2</sup>, the unscreened phonon frequencies of  $A_g(I)$  and  $A_g(II)$  modes are  $\omega_1 = (1/2.478)\sqrt{3K/2M} = 482$  cm<sup>-1</sup> and  $\omega_2 = \sqrt{3K/M} = 1690$  cm<sup>-1</sup>, respectively, 2.478 is the ratio of the  $C_{60}$  radius to the average bond length. The electron hopping is also fixed with value  $t_0 = 1.19$  eV. Figure 1 illustrates the dependence of the phonon frequencies on the  $e$ - $p$  coupling  $\lambda$ . The dashed and solid lines correspond to  $A_g(I)$  and  $A_g(II)$  modes, respectively. From the figure, we can see that the frequencies of two  $A_g$  modes first decrease as the  $e$ - $p$  coupling increases, then level off and begin to increase, and the change is more obvious for the bond-

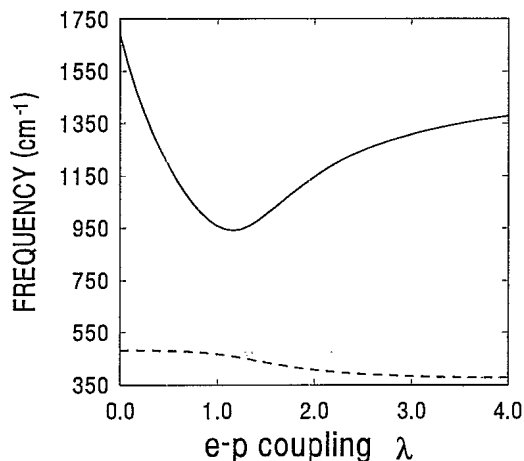


FIG. 1. The dependence of the frequencies of two  $A_g$  modes on the  $e$ - $p$  coupling  $\lambda$  when the electron correlation is absent, the dashed and solid lines represent  $A_g(I)$  and  $A_g(II)$  modes, respectively.

stretching mode  $A_g(II)$ . This evolution of the bond-stretching mode frequency as a function of the  $e$ - $p$  coupling is very different from the case in polyacetylene. In *trans*-polyacetylene, the ratio between the screened frequency  $\Omega$  and the unscreened one  $\omega$  of the bond-stretching mode is given by<sup>19</sup>

$$\Omega^2/\omega^2 = 2\lambda, \quad (14)$$

indicating that as  $\lambda \rightarrow 0$ ,  $\Omega$  goes to zero. But the zero frequency never occurs for any strength of the  $e$ - $p$  coupling in  $C_{60}$ . This difference can be understood if we notice that although both the  $C_{60}$  molecule and *trans*-polyacetylene favor a dimerization ground state, unlike polyacetylene, the dimerized ground state in  $C_{60}$  has no degeneracy. The effective potential of polyacetylene with different  $e$ - $p$  couplings in Fig. 2 shows that when the  $e$ - $p$  coupling is weak and the dimerization amplitude is small, the symmetrical potential well becomes shallow, and if  $\lambda$  tends to zero, the potential is flat and the effective force constant associated with the bond-stretching mode approaches zero. However, such feature cannot appear in the  $C_{60}$  since its ground state has no degeneracy. So, even if the  $e$ - $p$  coupling  $\lambda$  is zero and there is no dimerization in the ground state of  $C_{60}$ , the frequency of the bond-stretching mode  $A_g(II)$  is finite, taking the value of the unscreened phonon frequency  $\omega_2$ . The line shape of Fig. 1 is understandable when we are conscious of that in  $C_{60}$ , the  $e$ - $p$  coupling has two effects: on the one hand, it causes electron polarization to screen the ion-ion interaction and reduces the vibrational frequencies; on the other hand, it leads to the dimerization in the ground state and enlarges the gap between the lowest unoccupied molecular orbital (LUMO) and highest occupied molecular orbital (HOMO), weakening the polarization. The gap dependence on the  $e$ - $p$  coupling  $\lambda$  in  $C_{60}$  is shown in Fig. 3. When the  $e$ - $p$  coupling is weak, the first effect is dominant, while, when the  $e$ - $p$  coupling strength increases, the latter becomes more and more important. So the evolution of frequency as a function of  $\lambda$  is not monotonic.

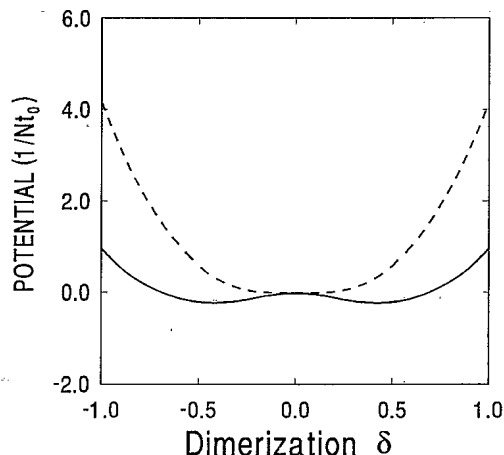


FIG. 2. The effective potential of polyacetylene as a function of the dimensionless dimerization amplitude  $\delta$ . The potential has a symmetry between  $\delta$  and  $-\delta$ . The solid and dashed lines correspond to  $\lambda = 0.1$  and  $0.05$ , respectively.

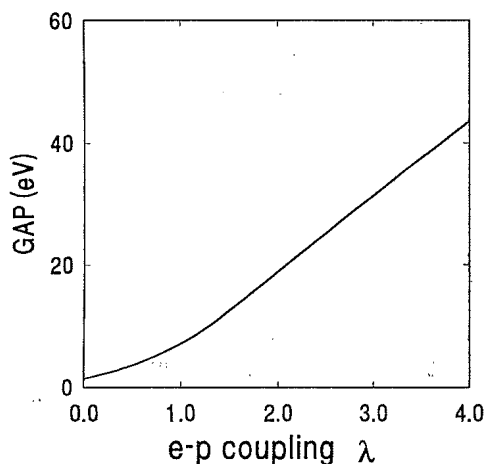


FIG. 3. The gap between the LUMO and HOMO in  $C_{60}$  as a function of the  $e$ - $p$  coupling  $\lambda$ .

The feature that the frequency change of the  $A_g(II)$  mode is more obvious than that of the  $A_g(I)$  mode is due to the bond-length-varying-type  $e$ - $p$  coupling in Hamiltonian (2), so the more influence is expected on the bond-stretching mode  $A_g(II)$ . However, in the vibration of the  $A_g(I)$  mode, the bond lengths can hardly be changed, and in this case, the  $e$ - $p$  coupling is not very serious.

In the different  $e$ - $p$  coupling regions, we have calculated the frequencies of the two modes including the correlation effect. The frequency of  $A_g(I)$  mode as a function of the Hubbard parameter  $U$  for different  $e$ - $p$  couplings is described in Fig. 4, and the dependence of the frequency of  $A_g(II)$  mode on  $U$  is illustrated in Fig. 5. Here, we select three  $e$ - $p$  coupling values,  $\lambda=0.198$ ,  $\lambda=1.446$ , and  $\lambda=3.174$ . From Fig. 1,  $\lambda=0.198$  is in the regime of  $e$ - $p$  coupling (named regime A), where both the frequencies of two  $A_g$  modes decrease as  $\lambda$  increases;  $\lambda=1.446$  is in the regime (named regime B), in which the frequency of  $A_g(I)$  mode decreases as  $\lambda$  increases, while, the frequency

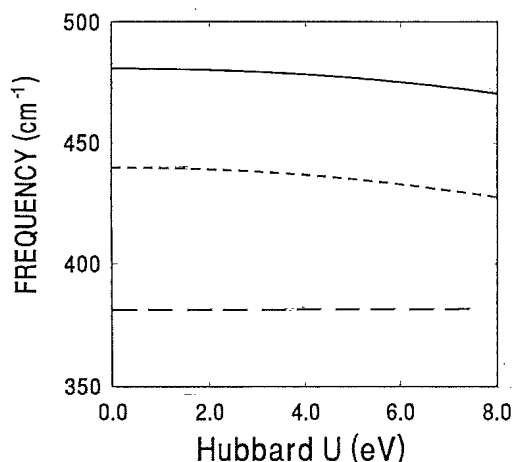


FIG. 4. The dependence of the frequency of  $A_g(I)$  mode on the Hubbard parameter  $U$  for three different values of  $e$ - $p$  coupling  $\lambda$ . The solid, short-dashed, and long-dashed lines correspond to  $\lambda=0.198$ , 1.446, and 3.174, respectively.

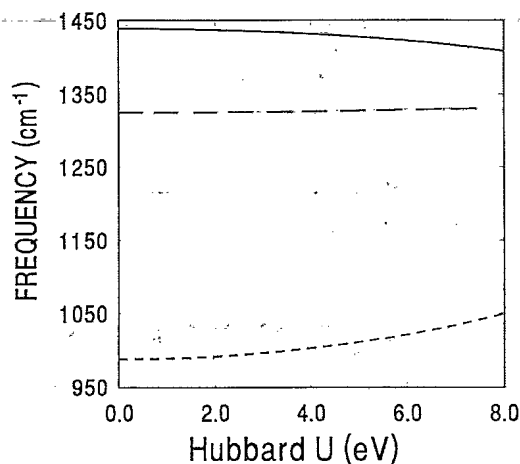


FIG. 5. The dependence of the frequency of the  $A_g(II)$  mode on the Hubbard parameter  $U$  for three different values of  $e$ - $p$  coupling  $\lambda$ . The solid, short-dashed, and long-dashed lines correspond to  $\lambda=0.198$ , 1.446, and 3.174, respectively.

of  $A_g(II)$  mode increases;  $\lambda=3.174$  is in the regime (named regime C), where both these frequencies increase as  $\lambda$  increases. We find that when the strength of  $e$ - $p$  coupling is small, electron correlation will reduce the frequencies of these modes; when the  $e$ - $p$  coupling is strong, electron correlation will increase their frequencies.

Since the 60 atoms in  $C_{60}$  with icosahedral symmetry are equivalent, on average, there is no double occupation at one site. In the Hartree-Fock approximation, the Hubbard repulsion has no effect on the  $A_g$  vibrational modes. Therefore, the frequency changes of these two modes come from the correlation effect. It is not easy to give a clear physical picture of how the electron correlation affects the vibration in the  $C_{60}$ , because of the many-body property of the correlation. According to the analysis of the valence bond diagram approach in polyacetylene by Mazumdar and Dixit, the correlation prevents the hopping between two neighboring sites.<sup>22</sup> Here we give an oversimplified picture by thinking that the correlation only reduces the hopping  $t_0$  to an effective one  $\tilde{t}_0 < t_0$ , and the correlation effect on two  $A_g$  modes in  $C_{60}$  can be understood by using the effective  $e$ - $p$  coupling  $\tilde{\lambda} \equiv 2\alpha^2 / (\pi K \tilde{t}_0) > \lambda$  and being aware of the dependence of the vibrational frequencies on the  $e$ - $p$  coupling. Thus, in regime A of  $e$ - $p$  coupling, where  $\lambda$  is small, the correlation reduces the two frequencies; in regime C, where  $\lambda$  is large, the correlation increases these frequencies, and in regime B with the intermediate  $e$ - $p$  coupling, the correlation decreases the frequency of the  $A_g(I)$  mode and increases the frequency of the  $A_g(II)$  mode. Figures 4 and 5 confirm this point. Having the aid of this picture, we can also easily explain why the correlation enhances the dimerization in polyacetylene and the length difference between the long and short bonds in  $C_{60}$ .<sup>19,20</sup>

In order to estimate the correlation effect for the real  $C_{60}$  molecule, we choose the realistic parameters used in Ref. 10, and the  $e$ - $p$  coupling  $\lambda=0.198$ . When the Hubbard repulsion is absent, these parameters yield the fre-

frequencies of  $481\text{ cm}^{-1}$  for the  $A_g(I)$  mode and  $1439\text{ cm}^{-1}$  for  $A_g(II)$  mode. With this relatively weak  $e$ - $p$  coupling, the correlation reduces the frequencies of two  $A_g$  modes. In the realistic region of the Hubbard parameter  $U$ , the change of frequency is not small when  $U$  increases from 0 to 8 eV,  $10\text{ cm}^{-1}$  for the  $A_g(I)$  mode and  $30\text{ cm}^{-1}$  for the  $A_g(II)$  mode, both these frequency shifts are much larger than the resolution of the Raman spectra experiment ( $<9\text{ cm}^{-1}$ ).<sup>21</sup> So the correlation effect must be taken into account to study the vibration in the  $C_{60}$ . The correlation effect on the frequencies of other vibrational modes can be roughly reckoned in accordance with our simplified physical picture, in which the correlation just renormalizes the  $e$ - $p$  coupling  $\lambda$ . Since the  $e$ - $p$  coupling is the most serious in the  $A_g(II)$  mode and the least serious in the  $A_g(I)$  one because of the bond-length-varying-type  $e$ - $p$  coupling in Su-Schrieffer-Heeger-like Hamiltonian, the reduction of the frequencies of other modes by the correlation should be situated between these two limits, i.e., larger than  $10\text{ cm}^{-1}$  but less than  $30\text{ cm}^{-1}$  at  $U=8\text{ eV}$ . The results of perturbation theory in Ref. 16 indicated that the phonon spectrum of neutral  $C_{60}$  is insensitive to the  $e$ - $e$  interaction, and surprisingly, the correlation has no effect on the full-symmetric  $A_g$  modes, which we believe is an artifact of their approximation scheme apart from perturbation theory.<sup>16</sup>

The accurate experimental results of the bond structure and the vibrational frequencies of two  $A_g$  modes in  $C_{60}$  are now available from the NMR techniques<sup>23</sup> and

Raman spectra,<sup>21</sup> 1.45 and  $1.40\text{ \AA}$  for the long and short bonds, 497 and  $1469\text{ cm}^{-1}$  for  $A_g(I)$  and  $A_g(II)$  modes. When the moderate  $U$  is included, the calculated bond lengths and vibrational frequencies cannot tally with above data if the parameters of Ref. 10 are used. Since the presence of the intermediate  $U$  in  $C_{60}$  has been widely accepted, we choose the strength of the Hubbard interaction with a typical intermediate value  $U=8\text{ eV}$  and determine other parameters by fitting the experimental data. The stiffness constant  $K$  can be obtained from the frequency of the  $A_g(I)$  mode since the effects of both the  $e$ - $p$  and  $e$ - $e$  interactions are not very obvious on this mode. From the numerical calculation, we know that the bond lengths are not sensitive to  $t_0$  but sensitive to  $\alpha$ , while both  $t_0$  and  $\alpha$  influence the vibrational frequencies, so  $\alpha$  can be obtained by fitting the bond lengths, afterwards  $t_0$  is determined from the frequencies. Finally, we have  $t_0=1.86\text{ eV}$ ,  $\alpha=5.3\text{ eV/\AA}$ ,  $K=46.4\text{ eV/\AA}^2$ , and these parameters yield the bond lengths 1.45 and  $1.40\text{ \AA}$ , the frequencies 494 and  $1469\text{ cm}^{-1}$ , which are very close to the experimental values.

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