ASITP

INSTITUTE OF THEORETICAL PHYSICS ACADEMIA SINICA

AS-ITP-94-01
January 1994

Fermilab Library
0 1160 0033172 2

ELECTRON–PHONON INTERACTION OF HIGH FREQUENCY MODE IN A_3C_{60}

Han–Ying GUO

Ming–Liang ZHANG

NAME | I D No. | M.S.

RETURN TO FERMILAB LIBRARY

MAR 15 1994

P.O.Box 2735, Beijing 100080, The People's Republic of China

Telefax : (86)-1-2562587 Telephone : 2568348

Telex : 22040 BAOAS CN Cable : 6158

$\mathcal{ASITP}$-94-01

Electron-Phonon Interaction Of High Frequency Mode In A_3C_{60}

Han-Ying Guo and Ming-Liang Zhang

CCAST (World Laboratory)
P. O. Box 8730, Beijing 100080, China

and

Institute of Theoretical Physics, Academia Sinica
P. O. Box 2735, Beijing 100080, China[1]

Abstract

The formula of λ of the crystal where one cell contains many components is derived in "nearly free" electron approximation. It is very important for the crystal in which one cell contains many components (for example A_3C_{60}). Old McMillan approximation is even given error predirect for these systems. The phase interferenes among these components can not be ignoreded. The electron-phonon interaction induced by the high frequency mode on ball is computed. It further prove the main part of electron-phonon interaction which resulted in superconductivity of A_3C_{60} is the part of low frequency mode of intermolecular.

Keywords:Highfrequency mode, electron-phonon interaction, interference.

submitted to Z.Physik B

[1]Mailing address

I. Introduction

Alkalis doped fulleren has been intensely investigated. Many author compute dimensionless electron-phonon coupling constant induced by high frequency on ball making use of McMillan approximation [1]

$$< \omega^2 > \; = \frac{\int_0^{\omega_{max}} \alpha^2 F(\omega)\omega d\omega}{\int_0^{\omega_{max}} \frac{1}{\omega}\alpha^2 F(\omega) d\omega} \approx \frac{\int_0^{\omega_{max}} F(\omega) d\omega}{\int_0^{\omega_{max}} \frac{1}{\omega} F(\omega) d\omega}. \tag{1}$$

Under this approximation it is easy to show [2,3]

$$\lambda = \sum_i \frac{N(0) < I_i^2 >}{M_i < \omega^2 >} \tag{2}$$

where i indicated ith component in one cell. However this formula exists serious error when use it to compute dimensionless electron-phonon coupling constant for the crystal in which one cell contains many components. About twenty years ago I.Gomersall and B.Gyorffy considered the electron-phonon mass enhancement in transition metal compounds, they given the phase shift method for λ of the crystal where one cell contains many components in muffin-tin approximation in appendix [2]. It is fit for the case where the scattering between ions and electrons is strong. They only used it to two components compound where the difference of mass between two components is very large. But the mass of C atoms on C_{60} is the same. The scattering between the carbon atom cores on ball and "nearly free" electrons in A_3C_{60} is not strong. In section II we first reconstruct the formula of λ for crystal in which one cell contain many components which fitting for A_3C_{60}. In section III we compute the electron-phonon interaction induced by high frequency mode on ball.

II. The general formulation of λ of many components crystal

λ is given

$$\lambda \; = \int \frac{d\omega}{\omega} \alpha^2 F(\omega) \tag{3}$$

where

$$\alpha^2 F(\omega) = \frac{V}{\hbar^2 (2\pi)^3} \sum_\nu \int_{S_F} \frac{d^2 k}{v_F} \int_{S_F} \frac{d^2 k'}{v_F} |\tilde{g}_{\nu,k',k}|^2 B_\nu(k'-k,\omega) / \int \frac{d^2 k}{v_F}, \tag{4}$$

in which V is crystal volume,

$$B_\nu(k'-k,\omega) = -\frac{1}{\pi} Im D_\nu(k'-k,\omega+i\delta) \tag{5}$$

is phonon spectrum function, $D_\nu(q,i\omega_\nu)$ is Fourier transformation of $D_\nu(q,\tau)$.

$$D_\nu(q,i\omega_\nu) = \frac{1}{\hbar\beta}\int_0^\beta d\tau e^{i\omega_n\tau} D_\nu(q,\tau)$$

$$D_\nu(q,\tau) = -<T_\tau A(q,\nu)A^+(q,\nu)>$$

, where

$$A_\nu(q,\nu) = a_{q,\nu} + a^+_{q,\nu}$$

. To compute $\alpha^2F(\omega)$ we first write perturbation potential of electron-phonon interaction

$$H_{el-ph} = \int \psi^\dagger(r)V_p(r)\psi(r)d^3r \tag{6}$$

where

$$\begin{aligned} V_p(r) &= -\textstyle\sum_{n,i,\alpha} u_{n,i,\alpha} \nabla_\alpha V_i(r-R_n-d_i) \\ \psi(r) &= \textstyle\sum_k \psi_k(r)c_k \end{aligned} \tag{7}$$

substituting above two formula to (13) we have

$$H_{el-ph} = -\int d^3r \textstyle\sum_{k,k'} \sum_{n,i,\alpha} \psi^*_{k'}(r) \nabla_\alpha V_i(r-R_n-d_i)\psi_k(r)u_{n,i,\alpha}c^\dagger_{k'}c_k \tag{8}$$

making use of the expression of displacement

$$u_{n,i,\alpha} = \textstyle\sum_{\nu,q}[\frac{\hbar}{2NM_i\omega_\nu(q)}]^{1/2}e^\nu_{i,\alpha}(q)e^{iqR_n}(a_{q,\nu}+a^\dagger_{-q,\nu}) \tag{9}$$

one can obtain

$$\begin{aligned} H_{el-ph} &= -\textstyle\sum_{k,k'}\sum_{\nu,q}\sum_{n,i,\alpha}\int d^3r[\frac{\hbar}{2NM_i\omega_\nu(q)}]^{1/2}\psi^*_{k'}(r) \\ &\quad \nabla_\alpha V_i(r-R_n-d_i)\psi_k(r)e^\nu_{i,\alpha}(q)e^{iqR_n}c^\dagger_{k'}c_k(a_{q,\nu}+a^\dagger_{-q,\nu}). \end{aligned} \tag{10}$$

According to Bloch theorem it can be written

$$\begin{aligned} H_{el-ph} &= -\textstyle\sum_{k,k'}\sum_{\nu,q}\sum_{n,i,\alpha}[\frac{\hbar}{2NM_i\omega_\nu(q)}]^{1/2}\int d^3r\psi^*_{k'}(r)\nabla_\alpha V_i(r-d_i) \\ &\quad \psi_k(r)e^{i(q+k+k')R_n}e^\nu_{i,\alpha}(q)c^\dagger_{k'}c_k(a_{q,\nu}+a^\dagger_{-q,\nu}) \end{aligned} \tag{11}$$

In terms of

$$\textstyle\sum_n e^{iR_n(q+k-k')} = \frac{(2\pi)^3}{\Omega}\sum_\ell \delta(q+k-k'-K_\ell) = \frac{(2\pi)^3}{\Omega}\delta(k+q-k') \tag{12}$$

we have

$$\begin{aligned} H_{el-ph} &= -\textstyle\sum_{\nu,k,k'}\sum_{i,\alpha}[\frac{\hbar}{2NM_i\omega_\nu(q)}]^{1/2}\int d^3r\psi^*_{k'}(r) \\ &\quad \nabla_\alpha V_i(r-d_i)\psi_k(r)e^\nu_{i,\alpha}(k'-k)c^\dagger_{k'}c_k(a_{k'-k,\nu}+a^\dagger_{-(k'-k),\nu}) \\ &= \textstyle\sum_{\nu,k',k}\tilde g_{\nu,k',k}c^\dagger_{k'}c_k(a_{k'-k,\nu}+a^\dagger_{-(k'-k),\nu}) \end{aligned} \tag{13}$$

in which

$$\tilde g_{k',k,\nu} = -\textstyle\sum_{i,\alpha}[\frac{\hbar}{2NM_i\omega_\nu(q)}]^{1/2}\int d^3r\psi^*_{k'}(r)\nabla_\alpha V_i(r-d_i)\psi_k(r)e^\nu_{i,\alpha}(k'-k) \tag{14}$$

So that

$$\begin{aligned} \alpha^2F(\omega) &= \textstyle\frac{V}{\hbar^2(2\pi)^3}\sum_{i,\alpha,j,\beta}\sum_\nu\int\frac{d^2k}{v_F}\int\frac{d^2k'}{v_F}\frac{\hbar}{2N\omega_\nu(k'-k)\sqrt{M_iM_j}} \\ &\quad \textstyle\int d^3r\psi^*_{k'}(r)\nabla_\alpha\tilde V_i(r-d_i)\psi_k(r)\int d^3r'\psi^*_k(r')\nabla_\beta\tilde V_j(r'-d_j)\psi_{k'}(r') \\ &\quad e^\nu_{i,\alpha}(k'-k)e^\nu_{j,\beta}(k'-k)[-\tfrac{1}{\pi}ImD_\nu(k'-k,\omega+i\delta)]/\int\tfrac{d^2k}{v_F} \\ &= -\textstyle\frac{V}{\hbar^2(2\pi)^3\pi}\sum_{i,\alpha,j,\beta}\int\frac{d^2k}{v_F}\int\frac{d^2k'}{v_F} \\ &\quad <k'|\nabla_\alpha\tilde V_i(r-d_i)|k><k|\nabla_\beta\tilde V_j(r'-d_j)|k'> \\ &\quad \textstyle\sum_\nu\frac{\hbar e^\nu_{i,\alpha}(k'-k)e^\nu_{j,\beta}(k'-k)}{2N\omega_\nu(k'-k)\sqrt{M_iM_j}}ImD_\nu(k'-k,\omega+i\delta)/\int\frac{d^2k}{v_F} \end{aligned} \tag{15}$$

here we account

$$D_{\alpha,\beta}(i,j,q;i\omega_n) = \sum_\nu\frac{\hbar e^\nu_{i,\alpha}(k'-k)e^\nu_{j,\beta}(k'-k)}{2N\omega_\nu(k'-k)\sqrt{M_iM_j}}D_\nu(k'-k,i\omega_\nu)$$

$$\begin{aligned} \alpha^2F(\omega) &= -\textstyle\frac{V}{\hbar^2(2\pi)^3\pi}\sum_{i,\alpha,j,\beta}\int\frac{d^2k}{v_F}\int\frac{d^2k'}{v_F}<k'|\nabla_\alpha\tilde V_i(r-d_i)|k> \\ &\quad <k|\nabla_\beta\tilde V_j(r'-d_j)|k'>ImD_{\alpha,\beta}(i,j,q;i\omega_n)/\int\tfrac{d^2k}{v_F} \end{aligned} \tag{16}$$

Making use of

$$2\int\tfrac{d\omega}{\omega}ImD_{\alpha,\beta}(i,j,q;i\omega_n) = \pi D_{\alpha,\beta}(i,j,q;i\omega_n=0) \tag{17}$$

$$\lambda = 2\int \frac{\alpha^2 F(\omega)}{\omega} d\omega = -\frac{V}{\hbar^2(2\pi)^3} \sum_{i,\alpha,j,\beta} \int \frac{d^2k}{v_F} \int \frac{d^2k'}{v_F}$$
$$< k'| \nabla_\alpha \tilde{V}_i(r-d_i)|k >< k| \nabla_j \tilde{V}_j(r'-d_j)|k' > D_{\alpha,\beta}(i,j,q;i\omega_n=0)$$
$$= -\frac{V}{\hbar^2(2\pi)^3} \frac{1}{N} \sum_{i,\alpha,j,\beta} \sum_{R_\ell - R_{\ell'}} \int \frac{d^2k}{v_F} \int \frac{d^2k'}{v_F} < k'| \nabla_\alpha \tilde{V}_i(r-d_i)|k >$$
$$< k| \nabla_\beta \tilde{V}_j(r'-d_j)|k' > D_{\alpha,\beta}(\ell,i,\ell' j;i\omega_n=0) e^{-iq(R_\ell - R_{\ell'})} / \int \frac{d^2k}{v_F} \tag{18}$$

In appendix we have shown that the delocalized vibration is not important for electron-phonon interaction, therefore we can take approximation

$$D_{\alpha,\beta}(\ell,i,\ell',j;i\omega_n=0) = \delta_{\ell,\ell'} D_{\alpha,\beta}(\ell,i,\ell,j;i\omega_n=0) \tag{19}$$

so that

$$\lambda = -\frac{V}{\hbar^2(2\pi)^3} \frac{1}{N} \sum_{i,\alpha,j,\beta} \int \frac{d^2k}{v_F} \int \frac{d^2k'}{v_F} < k'| \nabla_\alpha \tilde{V}_i(r-d_i)|k >$$
$$< k| \nabla_\beta \tilde{V}_j(r'-d_j)|k' > D_{\alpha,\beta}(\ell,i,\ell,j;i\omega_n=0) / \int \frac{d^2k}{v_F} \tag{20}$$

In appendix we prove

$$D_{\alpha,\beta}(\ell,i,\ell',j;i\omega_n=0) = -\hbar[\Phi]^{-1}_{\ell,i,\alpha;\ell',j,\beta} \tag{21}$$

λ is written

$$\lambda = \frac{V}{\hbar(2\pi)^3} \frac{1}{N} \sum_{i,\alpha,j,\beta} \Phi^{-1}_{\ell,i,\alpha;\ell,j,\beta} M^{i,j}_{\alpha,\beta} / \int \frac{d^2k}{v_F} \tag{22}$$

$$\lambda = \frac{\Omega_\alpha}{\hbar(2\pi)^3} \sum_{i,\alpha} \Phi^{-1}_{\ell,i,\alpha;\ell,i,\alpha} M^{ii}_{\alpha,\alpha} / \int \frac{d^2k}{v_F} +$$
$$\frac{\Omega_\alpha}{\hbar(2\pi)^3} \sum_{i,\alpha,j} \Phi^{-1}_{\ell,i,\alpha;\ell,j,\alpha} M^{ij}_{\alpha,\alpha} / \int \frac{d^2k}{v_F} \tag{23}$$

$$M^{i,j}_{\alpha,\beta} = \int \frac{d^2k}{v_F} \int \frac{d^2k'}{v_F} < k'| \nabla_\alpha \tilde{V}_i(r-d_i)|k >< k| \nabla_\beta \tilde{V}_j(r'-d_j)|k' > \tag{24}$$

III. Conclusions

In our previous paper [5,6] we have assumed the electron-phonon interaction induced by intra-molecule high frequency vibration modes is weaker than that of low frequency modes of inter-molecule for A_3C_{60} (the A^+ optical mode and the mass center vibration of C_{60}^{2-}).

For A_3C_{60} we apply above formula computing the contribution of high frequency vibration mode on ball for electron-phonon interaction. If noticing the ionized energy of carbon is eV, we can approximate the effective nuclear charge of C atoms equal to 1.82(hydrogenlike approximation) . We have prove in [6] the configuration of A_3C_{60} is every C_{60} carried two negative charge and there is one "nearly free" electron in every cell. For K_3C_{60}, the lattice constant is 14.25$\mathring{A}$, so the Fermi vector is $0.345 \times 10^{10}(m^{-1})$. Using frequency value and multiply of all modes list in Tab.1 and corresponding eigenvector of vibration, we obtain $\lambda = 3.94 \times 10^{-4}$, the sum of the contribution of individual atoms is $\lambda_1 = 5.17 \times 10^{-5}$, the contribution from interference among atoms $\lambda_2 = 3.41 \times 10^{-4}$. It is clear that the interference among atoms is important for crystal which one cell contain many component. This note proves the assumption in [5,6] is true.

Appendix

Let us mimic J.Apple and W.Kohn [4] writing phonon vertex in wannier representation for many components crystal

$$I_{ph}(n_1',n_2',n_1,n_2;\omega) = \sum_{p_1,p_1',p_2,p_2'} e^{i(p_1'n_1'+p_2'n_2'-p_1n_1-p_2n_2)} I_{ph}(p_1',p_2',p_1,p_2;\omega),$$
$$I_{ph}(p_1',p_2',p_1,p_2) = \sum_\nu g_\nu(p_1',p_1) g_\nu(p_2',p_2) D_\nu(p_1'-p_1) \delta_{p_1'-p_1,p_2-p_2'}, \tag{25}$$

where n_1', n_2', n_1, n_2 are lattice sites indexes, and $g_\nu(p_1',p_1)$ and $g_\nu(p_1',p_1)$ are matrix element for emission and absorption a phonon with momentum $q = p_1' - p_1$ respectively,

$$g_\nu(p_1',p_1) = -\sum_{n,i,\alpha} \left(\frac{1}{2NM_i\omega_\nu(q)}\right)^{1/2} e^{(\nu)}_{i\alpha}(q) e^{iqR_n} \int \psi^*_{p_1'}(r) \nabla_\alpha V_i(r-R_n-d_i) \psi_{p_1}(r) d^3r$$
$$= -\sum_{nia,s_1,s_1'} \left(\frac{1}{2NM_i\omega_\nu(q)}\right)^{1/2} e^{(\nu)}_{i\alpha}(q) e^{-iqR_n} e^{i(-p_1's_1'+p_1s_1)}$$
$$\frac{1}{N} \int w^*(r-R_{s_1'}) \nabla_\alpha V_i(r-R_n-d_i) w(r-R_{s_1}) d^3r, \tag{26}$$

where $w(r-s_1)$ is wannier function which center is at s_1th cell. The cell is composed of one C_{60} and three A^+, C_{60} is at center of rhombic dodecahedron consisted of fourteen

A^+.

$$
\begin{aligned}
g_\nu(p_2', p_2) &= -\sum_{mj\beta}\left(\frac{1}{2NM_j\omega_\nu(q)}\right)^{1/2} e^{(\nu)}_{j\beta}(q) e^{-iqR_m} \\
&\int \psi^*_{p_2'}(r')\, \nabla_\beta\, V_i(r' - R_m - d_j)\psi_{p_2}(r') d^3r' \\
&= -\sum_{mj\beta, s_2, s_2'}\left(\frac{1}{2NM_j\omega_\nu(q)}\right)^{1/2} e^{(\nu)}_{j\beta}(q) e^{-iqR_m} e^{i(-p_2' s_2' + p_2 s_2)} \\
&\quad \frac{1}{N}\int w^*(r' - R_{s_2'})\, \nabla_\beta\, V_j(r - R_m - d_j) w(r' - R_{s_2}) d^3r'.
\end{aligned}
\tag{27}
$$

$D_\nu(p_1' - p_1)$ is the phonon Green's function

$$
D_\nu(q) = \frac{2\omega_\nu(q)}{[\omega^2 - \omega_\nu^2(q)]} \tag{28}
$$

ν is polarization index. So that

$$
\begin{aligned}
I_{ph}(n_1', n_2', n_1, n_2; \omega) &= \sum_{l,m}\sum_{i\alpha, j\beta} L_{i\alpha, j\beta}(m, \omega)(n_1' |\, \nabla_\alpha\, V_i(r - R_l - d_i)| n_1) \\
&\quad (n_2' |\, \nabla_\beta\, V_j(r' - R_{l-m} - d_j)| n_2)
\end{aligned}
\tag{29}
$$

where

$$
(n' |\, \nabla_\alpha\, V_i(r - R_l - d_i)| n) = \int w^*(r - R_{n'})\, \nabla_\alpha\, V(r - R_l - d_i) w(r - R_n) d^3r, \tag{30}
$$

the matrix is small unless all three site are near each other. $L_{i\alpha, j\beta}(m, \omega)$ is a lattice Green's function in site space,

$$
L_{i\alpha, j\beta}(m; \omega) = \frac{1}{N}\sum_{\nu, q} \frac{e^{(\nu)}_{i\alpha}(q) e^{(\nu)}_{j\beta}(q)}{2\sqrt{M_i M_j}\omega_\nu(q)} D_\nu(q, \omega) e^{-iqR_m} \tag{31}
$$

It is negligible for $|m| >> a$, where a is lattice constant. Therefore $I_{ph}(n_1', n_2', n_1, n_2; \omega)$ is significant only when all four site variables are near each other. Above facts show it is localized vibrations that play important role in electron-phonon interaction, the long wavelength phonon is not important for electron-phonon interaction.

The phonon Green's function is

$$
\begin{aligned}
D_{\alpha,\beta}(\ell, i; \ell', j; \tau) &= D_{\alpha,\beta}(\ell - \ell', i; 0, j; \tau) = -\langle T_\tau u_{\alpha, \ell-\ell', i}(\tau) u_{\beta, 0, j}(0)\rangle \\
&= -\langle T_\tau u_{\alpha,\ell,i}(\tau) u_{\beta,\ell',j}(0)\rangle \\
&= \sum_{\nu,q}\sum_{\nu',q'}\left[\frac{\hbar}{2NM_i\omega_\nu(q)}\right]^{1/2}\left[\frac{\hbar}{2NM_j\omega_{\nu'}(q')}\right]^{1/2} e^{i(qR_\ell + q'R_{\ell'})} e^\nu_{\alpha,i}(q) e^{\nu'}_{\beta,j}(q') \\
&\qquad [-\langle T_\tau(a_{q,\nu}(\tau) + a^\dagger_{-q,\nu}(\tau))(a_{q',\nu'} + a^\dagger_{-q',\nu'})\rangle] \\
&= \sum_{\nu,q}\sum_{\nu',q'}\left[\frac{\hbar}{2NM_i\omega_\nu(q)}\right]^{1/2}\left[\frac{\hbar}{2NM_j\omega_{\nu'}(q')}\right]^{1/2} e^{i(qR_\ell + q'R_{\ell'})} e^\nu_{\alpha,i}(q) e^{\nu'}_{\beta,j}(q') \\
&\qquad [-\langle T_\tau(a_{q,\nu}(\tau) + a^\dagger_{-q,\nu}(\tau))(a_{q',\nu'} + a^\dagger_{-q',\nu'})\rangle] \\
&= \sum_{\nu,q}\sum_{\nu',q'}\left[\frac{\hbar}{2NM_i\omega_\nu(q)}\right]^{1/2}\left[\frac{\hbar}{2NM_j\omega_{\nu'}(q')}\right]^{1/2} e^{i(qR_\ell + q'R_{\ell'})} e^\nu_{\alpha,i}(q) e^{\nu'}_{\beta,j}(q') \\
&\qquad [-\langle T_\tau(a_{q,\nu}(\tau) + a^\dagger_{-q,\nu}(\tau))(a_{-q,\nu} + a^\dagger_{q,\nu})\rangle]\delta_{\nu,\nu'}\delta_{-q',q} \\
&= \sum_{\nu,q}\frac{\hbar}{2N\omega_\nu(q)\sqrt{M_i M_j}} e^{iq(R_\ell - R_{\ell'})} e^\nu_{\alpha,i}(q) e^\nu_{\beta,j}(q) \\
&\qquad [-\langle T_\tau A_\nu(q,\tau) A_\nu(-q, 0)\rangle] \\
&= \sum_{\nu,q}\frac{\hbar}{2N\omega_\nu(q)\sqrt{M_i M_j}} e^{iq(R_\ell - R_{\ell'})} e^\nu_{i,\alpha}(q) e^\nu_{j,\beta}(q) D_\nu(q,\tau)
\end{aligned}
\tag{32}
$$

$$
\begin{aligned}
D_{\alpha,\beta}(\ell, i; \ell', j; i\omega_n) &= \int_0^\beta e^{i\omega_n\tau} D_{\alpha,\beta}(\ell, i; \ell', j; \tau) \\
D_\nu(q, i\omega_n) &= \int_0^\beta e^{i\omega_n\tau} D_\nu(q,\tau)
\end{aligned}
$$

$$
\begin{aligned}
D_{\alpha,\beta}(\ell, i; \ell', j; i\omega_n) &= D_{\alpha,\beta}(\ell - \ell', i; 0, j; i\omega_n) \\
&= \sum_{\nu,q}\frac{\hbar e^{iq(R_\ell - R_{\ell'})} e^\nu_{\alpha,i}(q) e^\nu_{\beta,j}(q)}{2N\omega_\nu(q)\sqrt{M_i M_j}} D_\nu(q, i\omega_n) \\
&= \sum_{\nu,q}\frac{\hbar e^\nu_{i,\alpha}(q) e^\nu_{j,\beta}(q)}{2N\omega_\nu(q)\sqrt{M_i M_j}}\frac{2\omega_\nu(q)}{(i\omega_n)^2 - \omega_\nu^2(q)}
\end{aligned}
\tag{33}
$$

$$
D_{\alpha,\beta}(\ell, i; \ell', j; i\omega_n = 0) = -\sum_{\nu,q}\frac{\hbar e^\nu_{i,\alpha}(q) e^\nu_{j,\beta}(q)}{N\sqrt{M_i M_j}\omega_\nu^2(q)} e^{iq(R_\ell - R_{\ell'})} \tag{34}
$$

The dynamical matrix is

$$
\begin{aligned}
\Phi^{i,j}_{\alpha,\beta}(q) &= (M_i M_j)^{-1/2}\sum_{R_\ell - R_{\ell'}} \Phi_{\alpha,\beta;\ell,i;\ell',j} e^{-iq(R_\ell - R_{\ell'})} \\
\omega_\nu^2(q) e^\nu_{\alpha,i}(q) &= \sum_{\beta,j}\Phi_{\alpha,\beta;i,j}(q) e^{(\nu)}_{\beta,j}(q) \\
&= \sum_{\beta,j}\frac{1}{\sqrt{M_i M_j}}\sum_{R_\ell - R_{\ell'}} \Phi_{\alpha,\beta;\ell,i;\ell',j} e^{-iq(R_\ell - R_{\ell'})} e^{(\nu)}_{\beta,j}(q)
\end{aligned}
\tag{35}
$$

$$e^{\nu}_{\alpha,i}(q) = \sum_{\beta,j;R_\ell-R_{\ell'}} \frac{1}{\sqrt{M_iM_j}} e^{-iq(R_\ell-R_{\ell'})} \Phi_{\alpha,\beta;\ell,i;\ell',j} \frac{e^{\nu}_{\beta,j}(q)}{\omega^2_\nu(q)} \tag{36}$$

if one times $e^{\nu}_{\alpha',i'}(q)$ in two sides and sum over ν

$$\delta_{\alpha,\alpha'}\delta_{i,i'} = \sum_{\beta,j,R_\ell-R_{\ell'}} \frac{e^{-iq(R_\ell-R_{\ell'})}}{\sqrt{M_iM_j}} \sum_\nu \frac{e^{\nu}_{\alpha',i'}(q)e^{\nu}_{\beta,j}(q)}{\omega^2_\nu(q)} \Phi_{\alpha,\beta;\ell,i;\ell',j} \tag{37}$$

sum over q in two sides

$$N\delta_{\alpha,\alpha'}\delta_{i,i'} = \sum_{\beta,j,R_\ell-R_{\ell'}} \Phi_{\alpha,\beta;\ell,i;\ell',j} \sum_{q,\nu} \frac{e^{-iq(R_\ell-R_{\ell'})}}{\sqrt{M_iM_j}} \frac{e^{\nu}_{\alpha',i'}(q)e^{\nu}_{\beta,j}(q)}{\omega^2_\nu(q)} \tag{38}$$

$$\delta_{\alpha,\alpha'}\delta_{i,i'} = \sum_{\beta,j,R_\ell-R_{\ell'}} \Phi_{\alpha,\beta;\ell,i;\ell',j} \sum_{q,\nu} \frac{e^{-iq(R_\ell-R_{\ell'})}}{N\sqrt{M_iM_j}} \frac{e^{\nu}_{\alpha',i'}(q)e^{\nu}_{\beta,j}(q)}{\omega^2_\nu(q)} \tag{39}$$

$$\Phi^{-1}_{\alpha,\beta;\ell,i;\ell',j} = \sum_{q,\nu} \frac{e^{-iq(R_\ell-R_{\ell'})}e^{\nu}_{\alpha,i}(q)e^{\nu}_{\beta,j}(q)}{N\sqrt{M_iM_j\omega^2_\nu(q)}} \tag{40}$$

$$\Phi_{\alpha,\beta;\ell,i;\ell',j} = \left[\frac{\partial^2\Phi}{\partial u_{\alpha,\ell,i}\partial u_{\beta,\ell',j}}\right]_{u_{\alpha,\ell,i}=u_{\beta,\ell',j}=0} \tag{41}$$

$$D_{\alpha,\beta}(\ell,i;\ell';\omega=0) = [\Phi_{\alpha,\beta;\ell,i;\ell',j}]^{-1} \tag{42}$$

$$(\Phi^{-1})_{\alpha,\beta;i,j}(k-k') = \sum_\nu \frac{e^{\nu}_{i,\alpha}(k'-k)e^{\nu}_{j,\beta}(k'-k)}{\omega^2_\nu(k'-k)} \tag{43}$$

$$D_{\alpha,\beta}(\ell,i;\ell',j;i\omega_n) = \sum_{\nu,q} \frac{\hbar e^{\nu}_{i,\alpha}(q)e^{\nu}_{j,\beta}(q)e^{iq(R_\ell-R_{\ell'})}}{2N\sqrt{M_iM_j\omega_\nu(q)}} \frac{2\omega_\nu(q)}{(i\omega_n^2)-\omega^2_\nu(q)} \tag{44}$$

$$D_{\alpha,\beta}(\ell,i;\ell',j;i\omega_n=0) = -\sum_{\nu,q} \frac{\hbar e^{\nu}_{i,\alpha}(q)e^{\nu}_{j,\beta}(q)e^{iq(R_\ell-R_{\ell'})}}{N\sqrt{M_iM_j\omega^2_\nu(q)}} = -\hbar(\Phi^{-1})_{\ell,\alpha',i';\ell',\beta,j} \tag{45}$$

We calculated the electron-phonon matrix element, if we approximate dielectric function in Linard formula,

$$\begin{aligned} V_i(q) &= \frac{4\pi k Z_i e^2}{q^2\Omega_a} \\ \epsilon(q) &= k\frac{4me^2k_F}{\pi\hbar^2q^2} \\ \tilde{V}_i(q) &= \frac{\pi^2\hbar^2 Z_i}{\Omega_a m k_F} \end{aligned} \tag{46}$$

$$M^{i,j}_{\alpha,\beta} = \int_{S_F}\frac{d^2k}{v_F}\int_{S_F}\frac{d^2k'}{v_F} e^{i(k'-k)(d_i-d_j)}(k'-k)_\alpha(k'-k)_\beta V_i(k'-k)V_j(k'-k) \tag{47}$$

$$M^{i,i}_{x,x} = M^{i,i}_{y,y} = \frac{32\pi^2}{3}\left[\frac{\pi^4k_F^2Z^2\hbar^2}{\Omega_a}\right] \qquad M^{i,i}_{z,z} = \frac{16\pi^2}{3}\left[\frac{\pi^4k_F^2Z^2\hbar^2}{\Omega_a}\right] \tag{48}$$

$$\begin{aligned} M^{i,j}_{x,y} &= M^{i,j}_{x,z} = M^{i,j}_{y,z} = 0 \qquad M^{i,j}_{y,x} = M^{i,j}_{z,x} = M^{i,j}_{z,y} = 0 \\ M^{i,j}_{x,x} &= 32\pi^2\left[\frac{\pi^4k_F^2Z^2\hbar^2}{\Omega_a}\frac{sina(sina-acosa)}{a^4}\right] \\ M^{i,j}_{y,y} &= 32\pi^2\left[\frac{\pi^4k_F^2Z^2\hbar^2}{\Omega_a}\frac{sina(sina-acosa)}{a^4}\right] \\ M^{i,j}_{z,z} &= 32\pi^2\left[\frac{\pi^4k_F^2Z^2\hbar^2}{\Omega_a}\frac{-a^2cos2a+2asin2a+3cos2a-3}{a^4}\right] \end{aligned} \tag{49}$$

Acknowledgements

The authors would like to express their sincere gratitude to W.M.You, D.D.Yan, M.S.Miao, Y.Q.Liou, J.M.Lee, H.Y.Jin, H.T.Wang, S.J.Qin for their helpful discussions. We also wish to express our immense gratitude to W.M.You for suppling eigenvectors and corresponding eigenvalues of dynamical matrix and atom coordinates of C_{60}.

References

1. W.L.McMillan, Physical Review 167 (1968) 331.
2. I.R.Gomersall and B.L.Gyorffy, J.Phys.F:Metal Phys. 4 (1974) 1205.
3. D.W.Taylor and P.Vashishta, Physical Review B 5 (1972) 4410.
4. J.Appel and W.Kohn, Physical Review B 4 (1971) 2162.
5. M.L.Zhang and H.Y.Guo, (preprint) ASITP-93-60,CCAST-93-32, to appear in Acta Physica Sinica (in chinese).
6. M.L.Zhang and H.Y.Guo, (preprint) ASITP-93-61,CCAST-93-34, submitted to Physica C.