横场易兴模型的非线性效应*

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本文运用$n+1$时格林函数方法分析了横场易兴模型纵向极化过程的线性和非线性效应。推导出线性和非线性极化率以及检波、倍频、混频等非线性效应。说明了这些效应与隧道积分、互作用积分、频率、温度的依赖关系。

一、引　言

对KDP型铁电晶体和钙钛矿型铁电晶体的动态性质的研究不仅具有实用的价值。而且对研究铁电晶体的相变理论亦有重要的意义。对KDP型晶体的铁电相变目前普遍认为它属于有序—无序型[1]。而对钙钛矿型晶体的铁电相变是属于位移型或是有序—无序型或是介乎两者之间的类型目前仍未定论[2,3]。对于有序—无序型的铁电相变可以用横场易兴横型[4]很好地描写，本文指出对于用横场易兴模型描写的有序—无序系统的极化过程存在非线性效应。而位移型晶体极化过程没有非线性效应。因此利用极化过程是否存在非线性效应可作为区别有序—无序型或位移型铁电性的一个判据。

对有序—无序铁电晶体，我们采用横场易兴模型去描写，系统的哈密顿量表示为

$$\mathrm{H}=-\Omega\sum_{f}S_{f}^{x}-\frac{1}{2}\sum_{f_1f_2}J_{f_1f_2}S_{f_1}^{z}S_{f_2}^{z} \tag{1}$$

其中S_f为自旋算符，自旋算符的z分量S_f^z称为偶极矩算符，其统计平均值对应于系统的极化强度，自旋算符的x分量S_f^x称为隧道算符，其统计平均值对应系统的隧道效应。Ω为隧道积分，J为互作用积分。

研究系统的动态性质如在外电场作用下极化强度的变化我们采用$n+1$时格林函数方法，设系统的哈密顿

$$\mathrm{H}=\mathrm{H}_0+V(t) \tag{2}$$

其中H_0为系统未受微扰的哈密顿量，$V(t)$为外作用下的微扰能。

据文献[5]，系统的某一力学量A的统计平均值为

* 本文1978年11月收到。

$$\langle A(t)\rangle=\bar{A}+\sum_{n=1}^{\infty}\delta^{(n)}\langle A(t)\rangle \qquad (3)$$

(3)式中$\bar{A}$是系统未受微扰时A的统计平均值。

$\delta^{(n)}\langle A(t)\rangle$

$$=\sum_{\Omega_1\cdots\Omega_n}\iint_{-\infty}^{\infty}\cdots\iint dt_1\cdots dt_n G^{n+1}_{A;V_{\Omega_1}\cdots V_{\Omega_n}}(t-t_1,t_1-t_2,\cdots t_{n-1}-t_n)e^{\sum_{j=1}^{n}\varepsilon t_j-i\sum_{j=1}^{n}\Omega_j t_j}$$

$$=\sum_{\Omega_1\cdots\Omega_n}(2\pi)^n e^{-i\sum_{j=1}^{n}\Omega_j t+n\varepsilon t} G^{n+1}_{A;V_{\Omega_1}\cdots\Omega_n}\Big(\sum_{j=1}^{n}\Omega_j+in\varepsilon,\ \sum_{j=2}^{n}\Omega_j$$

$$+i(n-1)\varepsilon,\cdots\Omega_n+i\varepsilon\Big) \qquad (4)$$

其中　$V(t)=\sum_{\Omega}e^{\varepsilon t}e^{-i\Omega t}V_{\Omega}\ (\varepsilon\to 0^+)$

(4)式中$n+1$时推迟格林函数及其谱表示定义如下：

$$G^{n+1}_{A;V_{\Omega_1}\cdots V_{\Omega_n}}(t-t_1\cdots t_{n-1}-t_n)$$

$$=(-i)^n\theta(t-t_1)\theta(t_1-t_2)\cdots\theta(t_{n-1}-t_n)$$

$$\langle[\cdots[\widetilde{A}(t)\widetilde{V}_{\Omega_1}(t_1)]\widetilde{V}_{\Omega_2}(t_2)]\cdots\widetilde{V}_{\Omega_n}(t_n)]\rangle$$

$$=\iint_{-\infty}^{\infty}\cdots\iint dE_1dE_2\cdots dE_n\,G^{n+1}_{A;V_{\Omega_1}\cdots V_{\Omega_n}}(E_1E_2\cdots E_n)e^{-iE_1(t-t_1)-iE_2(t_1-t_2)\cdots\cdots-iE_n(t_{n-1}-t_n)}$$

其中　$\widetilde{A}(t)=e^{iH_0t}A(t)e^{-iH_0t}$，　$\widetilde{V}_{\Omega}(t)=e^{iH_0t}V_{\Omega}e^{-iH_0t}$

本文采用下面符号代表格林函数的谱表示

$$\langle\langle A|V_{\Omega_1}\|V_{\Omega_2}\|\!|\cdots V_{\Omega_n}\rangle\rangle_{E_1E_2\cdots E_n}=G^{n+1}_{A;V_{\Omega_1}\cdots V_{\Omega_n}}(E_1E_2\cdots E_n)$$

格林函数满足下述运动方程

$$E_1\langle\langle A|V_{\Omega_1}\|V_{\Omega_2}\|\!|\cdots V_{\Omega_n}\rangle\rangle_{E_1E_2\cdots E_n}=\frac{1}{2\pi}\langle\langle[AV_{\Omega_1}]|V_{\Omega_2}\|V_{\Omega_3}\|\!|\cdots V_{\Omega_n}\rangle\rangle_{E_2E_3\cdots E_n}$$

$$+\langle\langle[AH_0]|V_{\Omega_1}\|V_{\Omega_2}\|\!|\cdots V_{\Omega_n}\rangle\rangle_{E_1E_2\cdots E_n} \qquad (5)$$

利用(1)—(5)式可以计算系统在外电场作用下极化强度的变化。即极化过程的线性和非线性效应。

二、线性效应

本节主要计算线性极化率，我们讨论沿z轴外加电场极化的情形，这时(2)式中

$$V(t)=-\mu E_z\left(e^{-i\omega t}+e^{i\omega t}\right)\sum_f S_f^z. \tag{6}$$

E_z为沿z方向的外加电场强度，ω为电场振动园频率，μ为系统的元负载者 的有效电矩。

则元负载者的极化电矩为　$\mu\langle S_g^z\rangle$

物体的极化强度为$\langle P_z\rangle=\mu N_0\langle S_g^z\rangle$　　(7)

(7)式中N_0为单位体积内元负载者数，〈 〉表示统计平均值。

将(6)式(7)式代到(4)式，求出线性极化强度$\delta^{(1)}\langle P_z(t)\rangle$与外电场的关系。

$$\delta^{(1)}\langle P_z(t)\rangle=-\mu^2N.\ E_z\sum_f 2\pi\left\{\langle\langle S_g^z\,|S_f^z\rangle\rangle_\omega e^{-i\omega t}+\langle\langle S_g^z\,|S_g^z\rangle\rangle_{-\omega}e^{i\omega t}\right\} \tag{8}$$

据(5)式双时格林函数的运动方程为

$$\omega\langle\langle A|B\rangle\rangle_\omega=\frac{1}{2\pi}\langle[A\ B]\rangle+\langle\langle[A\ \mathbf{H}_0]|B\rangle\rangle_\omega \tag{9}$$

又根据自旋算符的对易关系

$$[S_g^x\ S_f^y]=iS_g^z\delta_{gf};\quad [S_g^y\ S_f^z]=iS_g^x\delta_{gf}\quad [S_f^z\ S_f^x]=iS_g^y\ \delta_{gf} \tag{10}$$

由(1)(9)(10)可得

$$\left.\begin{aligned}
&\omega\langle\langle S_g^z|S_f^z\rangle\rangle_\omega=-i\Omega\langle\langle S_g^y|S_f^z\rangle\rangle_\omega\\
&\omega\langle\langle S_g^y|S_f^z\rangle\rangle_\omega=\frac{i\langle S_g^x\rangle}{2\pi}\delta_{gf}+i\Omega\langle\langle S_g^z|S_f^z\rangle\rangle_\omega-i\sum_{f_1}J_{gf_1}\\
&\qquad\langle\langle S_g^x\ S_{f_1}^z|S_f^z\rangle\rangle_\omega\\
&\omega\langle\langle S_g^x|S_f^z\rangle\rangle_\omega=-\frac{i\langle S_g^y\rangle}{2\pi}\delta_{gf}+i\sum_{f_1}J_{gf_1}\langle\langle S_g^y\ S_{f_1}^z|S_f^z\rangle\rangle_\omega
\end{aligned}\right\} \tag{11}$$

据赝自旋系统是在沿x方向的隧道场，和沿z方向的互作用场作用下，因此$\langle S_g^y\rangle=0$

令　$\langle S_g^z\rangle=S$；　　$\langle S_g^x\rangle=x$．

求解(11)式作如下截断近似

$$\langle\langle S_g^x\ S_{f_1}^z|S_f^z\rangle\rangle=\langle S_g^x\rangle\langle\langle S_{f_1}^z|S_f^z\rangle\rangle+\langle S_{f_1}^z\rangle\langle\langle S_g^x|S_f^z\rangle\rangle$$

$$\langle\langle S_g^y\ S_{f_1}^zS|_{f_1}^z\rangle\rangle=\langle S_g^y\rangle\langle\langle S_{f_1}^z|S_f^z\rangle\rangle+\langle S_{f_1}^z\rangle\langle\langle S_g^y|S_f^z\rangle\rangle$$

(11)式变为

$$\left.\begin{aligned}
&\omega\langle\langle S_g^x|S_f^z\rangle\rangle_\omega=iSJ_0\langle\langle S_g^y|S_f^z\rangle\rangle_\omega\\
&\omega\langle\langle S_g^y|S_f^z\rangle\rangle_\omega=\frac{ix}{2\pi}\delta_{gf}+i\Omega\langle\langle S_g^z|S_f^z\rangle\rangle_\omega-iSJ_0\langle\langle S_g^x|S_f^z\rangle\rangle_\omega\\
&\qquad -ix\sum_{f_1}J_{gf_1}\langle\langle S_{f_1}^z|S_f^z\rangle\rangle_\omega\\
&\omega\langle\langle S_g^z|S_f^z\rangle\rangle_\omega=-i\Omega\langle\langle S_g^y|S_f^z\rangle\rangle_\omega
\end{aligned}\right\}\tag{12}$$

其中$J_0=\sum_f J_{gf}$

过渡到动量表象，对算符S_f作变换

$$S_f=\frac{1}{\sqrt{N}}\sum_q e^{-i(f,q)}S_q \tag{13}$$

由(13)式可得

$$\langle\langle S_g|S_f\rangle\rangle_\omega=\frac{1}{N}\sum_{qq_1}e^{-igq_1-ifq}\langle\langle S_{q_1}|S_q\rangle\rangle_\omega \tag{14}$$

据平移不变性

$$\langle\langle S_g|S_f\rangle\rangle_\omega=\langle\langle S_0|S_{f-g}\rangle\rangle_\omega=\frac{1}{N}\sum_{qq_1}e^{-i(f-g,p)}\langle\langle S_{q_1}|S_q\rangle\rangle_\omega \tag{15}$$

由(14)(15)式可得 $q_1=-q$

∴ $$\langle\langle S_g|S_f\rangle\rangle_\omega=\frac{1}{N}\sum_q e^{i(g-f,q)}\langle\langle S_{-q}|S_g\rangle\rangle_\omega \tag{16}$$

(16)式表示了平移不变性导至赝自旋波散射过程的动量守恒。

据(16)式，(12)式写成

$$\left.\begin{aligned}
&\omega\langle\langle S_{-q}^x|S_q^z\rangle\rangle_\omega=iSJ_0\langle\langle S_{-q}^z|S_q^z\rangle\rangle_\omega\\
&\omega\langle\langle S_{-q}^y|S_q^z\rangle\rangle_\omega=\frac{ix}{2\pi}+i\Omega\langle\langle S_{-q}^z|S_q^z\rangle\rangle_\omega-iSJ_0\langle\langle S_{-q}^x|S_q^z\rangle\rangle_\omega-\\
&\qquad -ixJ(q)\langle\langle S_{-q}^z|S_q^z\rangle\rangle_\omega\\
&\omega\langle\langle S_{-q}^z|S_q^z\rangle\rangle_\omega=-i\Omega\langle\langle S_{-q}^y|S_q^z\rangle\rangle_\omega
\end{aligned}\right\}\tag{17}$$

上面利用了 $\delta_{qf}=\frac{1}{N}\sum_q e^{i(g-f,q)}$

$$J(q)=\sum_{f_1}J_{gf_1}e^{i(f_1-g,q)}$$

(17)式的解为

$$\left.\begin{aligned}\langle\langle S^x_{-q}|S^z_q\rangle\rangle_\omega &= -\frac{1}{2\pi}\frac{xSJ_0}{\omega^2-\omega_q^2}\\ \langle\langle S^y_{-q}|S^z_q\rangle\rangle_\omega &= \frac{i}{2\pi}\frac{x\omega}{\omega^2-\omega_q^2}\\ \langle\langle S^z_{-q}|S^z_q\rangle\rangle_\omega &= \frac{1}{2\pi}\frac{x\Omega}{\omega^2-\omega_q^2}\end{aligned}\right\}\tag{18}$$

其中　$\omega_q^2 = S^2 J_0^2 + \Omega[\Omega - xJ(q)]$

据(8)式和(16)式可得

$$\delta^{(1)}\langle p_z(t)\rangle = -\mu^2 N_1 E_z 2\pi \langle\langle S_0^z|S_0^z\rangle\rangle_\omega (e^{-i\omega t}+e^{i\omega t})\tag{19}$$

将(18)式代入(19)式可得

$$\delta^{(1)}\langle p_z(t)\rangle = -\frac{\mu^2 N_0 x\Omega}{\omega^2-\omega_0^2}E_z(e^{-i\omega t}+e^{i\omega t})\tag{20}$$

其中　$\omega_0^2 = S^2J_0^2+\Omega(\Omega-xJ_0)$ 为软模频率。

由(20)式得线性极化率

$$\chi = -\frac{\mu^2N_0x\Omega}{\omega^2-\omega_0^2}\tag{21}$$

(21)式中的 x 和 S 由文献[6]给出的方程组确定。

对铁电相，$x=\frac{\Omega}{J_0}$；对顺电相，$\frac{\Omega}{J_0}$ 小于 $\frac{1}{2}$ 时，$x=\frac{\Omega}{J_0}\frac{\theta_c}{\theta}$。

(21)式给出 χ 与频率的关系当 $\omega=\omega_0$ 时 $\chi\to\infty$ 这时发生铁电共振吸收当考虑到系统的弛豫过程时 $\omega=\omega_0$ 时 χ 为有限值。上面给出 x 与温度的关系，当温度趋近转变温度时，$\theta\to\theta_c$；$S\to0$（铁电相）；$x\to\frac{\Omega}{J_0}$（顺电相）；$\omega_0\to0$，

三、非线性效应

1° 二倍频和检波效应：

设外界微扰能仍如(6)式，将(6)(7)式代到(4)式可求出检波项和二倍频项为

$$\delta^{(2)}\langle p_z(t)\rangle = \mu^3N_0E_z^2\sum_{f_1 f}(2\pi)^2\Big\{\langle\langle S_g^z|S_{f_1}^z\|S_f^z\rangle\rangle_{0,\omega}+\langle\langle S_g^z|S_{f_1}^z\|S_f^z\rangle\rangle_{0,-\omega}$$

$$+\langle\langle S_g^z|S_{f_1}^z\|S_f^z\rangle\rangle_{2\omega,\omega}e^{-i2\omega t}+\langle\langle S_g^z|S_{f_1}^z\|S_f^z\rangle\rangle_{-2\omega,-\omega}e^{i2\omega t}\Big\} \quad (22)$$

据（5）式可得三时格林函数的运动方程为

$$2\omega\langle\langle A|B\|C\rangle\rangle_{2\omega,\omega}=\frac{1}{2\pi}\langle\langle[AB]|C\rangle\rangle_{\omega}+\langle\langle[A\mathrm{H}_0]|B\|C\rangle\rangle_{2\omega,\omega} \quad (23)$$

据(1)(23)式，再利用自旋算符的对易关系和上面所用的截断近似，可得

$$\left.\begin{aligned}
2\omega\langle\langle S_g^x|S_{f_1}^z\|S_f^z\rangle\rangle_{2\omega,\omega}&=-\frac{i}{2\pi}\delta_{gf_1}\langle\langle S_g^y|S_f^z\rangle\rangle_{\omega}+iSJ_0\langle\langle S_g^y|S_{f_1}^z\|S_f^y\rangle\rangle_{2\omega,\omega}\\
2\omega\langle\langle S_g^y|S_{f_1}^z\|S_f^z\rangle\rangle_{2\omega,\omega}&=\frac{i}{2\pi}\delta_{gf_1}\langle\langle S_g^x|S_f^z\rangle\rangle_{\omega}+i\Omega\langle\langle S_g^z|S_{f_1}^z\|S_f^z\rangle\rangle_{2\omega,\omega}\\
&\quad-iSJ_0\langle\langle S_g^x|S_{f_1}^z\|S_f^z\rangle\rangle_{2\omega,\omega}-ix\sum_{f_2}J_{gf_2}\langle\langle S_{f_2}^z|S_{f_1}^z\|S_f^z\rangle\rangle_{2\omega,\omega}\\
2\omega\langle\langle S_g^z|S_{f_1}^z\|S_f^z\rangle\rangle_{2\omega,\omega}&=-i\Omega\langle\langle S_g^y|S_{f_1}^z\|S_f^z\rangle\rangle_{2\omega,\omega}
\end{aligned}\right\} \quad (24)$$

如(13)式将算符作变换，过渡到动量表象，如前面一样根据平移对称性可证明

$$\langle\langle S_g|S_{f_1}\|S_f\rangle\rangle_{2\omega,\omega}=\frac{1}{N^{\frac{3}{2}}}\sum_{qq_1}e^{i(g-f_1)+i(g-f,q)}\langle\langle S_{-q_1-q}|S_{q_1}\|S_q\rangle\rangle_{2\omega,\omega} \quad (25)$$

将(25)式代入(24)式，利用$\delta_{gf_1}=\frac{1}{N}\sum_{q_1}e^{(ig-f_1,q_1)}$和$J(q+q_1)=\sum_{f_2}J_{gf_2}e^{i(f_2-g,q_1+q)}$

可得

$$\left.\begin{aligned}
2\omega\langle\langle S_{-q_1-q}^x|S_{q_1}^z\|S_{q_2}^z\rangle\rangle_{2\omega,\omega}&=-\frac{i}{2\pi N^{\frac{1}{2}}}\langle\langle S_{-q}^y|S_q^z\rangle\rangle_{\omega}\\
&\quad+iSJ_0\langle\langle S_{-q_1-q}^y|S_{q_1}^z\|S_q^z\rangle\rangle_{2\omega,\omega}\\
2\omega\langle\langle S_{-q_1-q}^y|S_{q_1}^z\|S_q^z\rangle\rangle_{2\omega,\omega}&=\frac{i}{2\pi N^{\frac{1}{2}}}\langle\langle S_{-q}^x|S_q^z\rangle\rangle_{\omega}\\
&\quad+i\Omega\langle\langle S_{-q_1-q}^z|S_{q_1}^z\|S_q^z\rangle\rangle_{2\omega,\omega}\\
-iSJ_0\langle\langle S_{-q_1q}^x|S_{q_1}^z\|S_q^z\rangle\rangle_{2\omega,\omega}&-ixJ(q+q_1)\langle\langle S_{-q_1-q}^z|S_{q_1}^z\|S_z^q\rangle\rangle_{2\omega,\omega}\\
2\omega\langle\langle S_{-q_1-q}^z|S_{q_1}^z\|S_q^z\rangle\rangle_{2\omega,\omega}&=-i\Omega\langle\langle S_{-q_1-q}^y|S_{q_1}^z|S_q^z\rangle\rangle_{2\omega,\omega}
\end{aligned}\right\} \quad (26)$$

将(18)式代入(26)式可求得

$$\langle\langle S_{-q_1-q}^x|S_{q_1}^z\|S_q^z\rangle\rangle_{2\omega,\omega}=\frac{x}{2(2\pi)^2N^{\frac{1}{2}}}\frac{\{(2\omega)^2+2S^2J_0^2-\Omega[\Omega-xJ(q+q_1)]\}}{(\omega^2-\omega_q^2)[(2\omega)^2-\omega_{q+q_1}^2]}$$

$$\langle\!\langle S^y_{-q_1-q}|S^z_{q_1}\|S^z_q\rangle\!\rangle_{2\omega,\omega}=-\frac{i}{(2\pi)^2}\frac{3xSJ_0\omega}{N^{\frac{1}{2}}(\omega^2-\omega_q^2)[(2\omega)^2-\omega^2_{q+q_1}]}$$

$$\langle\!\langle S^z_{-q_1-q}|S^z_{q_1}\|S^z_q\rangle\!\rangle_{2\omega,\omega}=-\frac{3x\Omega SJ_0}{2(2\pi)^2N^{\frac{1}{2}}(\omega^2-\omega_q^2)[(2\omega)^2-\omega^2_{q+q_1}]} \tag{27}$$

将(25)(27)式代入到(22)式得到

倍频项 $\delta^{(2)}\langle P_z(t)\rangle_{倍}=\mu^3N_0(2\pi)^2N^{-\frac{1}{2}}\langle\!\langle S_0^z|S_0^z\|S_0^z\rangle\!\rangle_{2\omega,\omega}E_z^2(e^{-i2\omega t}+e^{i2\omega t})$

$$=-\frac{3\mu^3N_0x\Omega SJ_0}{2(\omega^2-\omega_0^2)[(2\omega)^2-\omega_0^2]}E_z^2(e^{-i2\omega t}+e^{i2\omega t}) \tag{28}$$

检波项 $\delta^{(2)}\langle P_z(t)\rangle_{检}=2\mu^3N_0(2\pi)^2N^{-\frac{1}{2}}\langle\!\langle S_0^z|S_0^z\|S_0^z\rangle\!\rangle_{0,\omega}E_z^2$

$$=\frac{3\mu^3N_0x\Omega SJ_0}{\omega_0^2(\omega^2-\omega_0^2)}E_z^2 \tag{29}$$

(28)(29)式表明在一般情况下倍频效应和检波效应比线性极化效应小很多，只当$\omega\approx\omega_0$时，软模被强烈地激发即发生铁电共振时，倍频和检波效应显著增强，或当$2\omega\approx\omega_0$亦有很强的倍频效应。(28)(29)式表明顺电相时因$S=0$，故不存在倍频和检波效应。

2° 和频和差频效应：

设外界微扰

$$V(t)=-\mu E_{1z}(e^{-i\omega_1t}+e^{i\omega_1t})\sum_f E_f^z-\mu E_{2z}(e^{-i\omega_2t}+e^{i\omega_2t})\sum_f S_f^z \tag{30}$$

类似1°的推导可得

和频效应：

$$\delta^{(2)}\langle P_z(t)\rangle_{和}=-\frac{3\mu^3N_0x\Omega SJ_0(\omega_1^2+\omega_2^2-2\omega_0^2)E_{1z}E_{2z}(e^{-i(\omega_1+\omega_2)t}+e^{i(\omega_1+\omega_2)t})}{2(\omega_1^2-\omega_0^2)(\omega_2^2-\omega_0^2)[(\omega_1+\omega_2)^2-\omega_0^2]} \tag{31}$$

差频效应：

$$\delta^{(2)}\langle P_z(t)\rangle_{差}=-\frac{3\mu^3N_0x\Omega SJ_0(\omega_1^2+\omega_2^2-2\omega_0^2)E_{1z}E_{2z}(e^{-i(\omega_1-\omega_2)t}+e^{i(\omega_1-\omega_2)t})}{2(\omega_1^2-\omega_0^2)(\omega_2^2-\omega_0^2)[(\omega_1-\omega_2)^2-\omega_0^2]} \tag{32}$$

(31)式表明当$\omega_1\cong\omega_0$；或$\omega_2\approx\omega_0$或$\omega_1+\omega_2\approx\omega_0$时，和频效应显著增强。

(32)式表明，当$\omega_1\approx\omega_0$，或$\omega_2\approx\omega_0$，或$\omega_1-\omega_2\approx\omega_0$时，差频效应显著增强。(31)(32)式表明顺电相时，因$s=0$，故不存在和频及差频效应。

3° 三倍频效应：

设外界微扰仍为(6)式所示。将(6)(7)式代入(4)式可得三倍频的极化强度与外电场

的关系：

$$\delta^{(3)}\langle P_z(t)\rangle = -\mu^4 N_0 E_z^3 \sum_{f_2 f_1 f} (2\pi)^3 \{ \langle\langle S_g^z | S_{f_2}^z \| S_{f_1}^z ||| S_f^z \rangle\rangle_{3\omega,2\omega,\omega} e^{-i3\omega t}$$

$$+ \langle\langle S_g^z | S_{f_2}^z \| S_{f_1}^z ||| S_f^z \rangle\rangle_{-3\omega,-2\omega,-\omega} e^{i3\omega t} \} \quad (33)$$

据(5)式四时格林函数的运动方程

$$3\omega \langle\langle A|B\|C|||D\rangle\rangle_{3\omega,2\omega,\omega} = \frac{1}{2\pi}\langle\langle [AB]|C\|D\rangle\rangle_{2\omega,\omega}$$

$$+ \langle\langle [AH_0]|B\|C|||D\rangle\rangle_{3\omega,2\omega,\omega} \quad (34)$$

再利用自旋算符的对易关系和上面所用的截断近似，并据(34)式可得

$$\left.\begin{aligned}
&3\omega \langle\langle S_g^x | S_{f_2}^z \| S_{f_1}^z ||| S_f^z \rangle\rangle_{3\omega,2\omega,\omega} = -\frac{i}{2\pi}\delta_{gf_2}\langle\langle S_g^y | S_{f_1}^z \| S_f^z \rangle\rangle_{2\omega,\omega} \\
&\quad + iSJ_0 \langle\langle S_g^y | S_{f_2}^z \| S_{f_1}^z ||| S_f^z \rangle\rangle_{3\omega,2\omega,\omega} \\
&3\omega \langle\langle S_g^y | S_{f_2}^z \| S_{f_1}^z ||| S_f^z \rangle\rangle_{3\omega,2\omega,\omega} = \frac{i}{2\pi}\delta_{gf_2}\langle\langle S_g^x | S_{f_1}^z \| S_f^z \rangle\rangle_{2\omega,\omega} \\
&\quad + i\Omega \langle\langle S_g^z | S_{f_2}^z \| S_{f_1}^z ||| S_f^z \rangle\rangle_{3\omega,2\omega,\omega} \\
&-iSJ_0 \langle\langle S_g^x | S_{f_2}^z \| S_{f_1}^z ||| S_f^z \rangle\rangle_{3\omega,2\omega,\omega} - ix \sum_{f_3} J_{gf_3} \langle\langle S_{f_3}^z | S_{f_2}^z | S_{f_1}^z ||| S_f^z \rangle\rangle_{3\omega,2\omega,\omega} \\
&3\omega \langle\langle S_g^z | S_{f_2}^z \| S_{f_1}^z ||| S_f^z \rangle\rangle_{3\omega,2\omega,\omega} = -i\Omega \langle\langle S_g^y | S_{f_2}^z \| S_{f_1}^z ||| S_f^z \rangle\rangle_{3\omega,2\omega,\omega}
\end{aligned}\right\} \quad (35)$$

如(13)式，将算符作变换，过渡到动量表象，如前面一样根据平移对称性可证明

$$\langle\langle S_g | S_{f_2} \| S_1 ||| S_f \rangle\rangle_{3\omega,2\omega,\omega} = \frac{1}{N^2}\sum_{qq_1q_2} e^{i(g-f,q)+i(g-f_1q_1)+i(g-f_2q_2)}$$

$$\langle\langle S_{-g-q_1-q_2} | S_{q_2} \| S_{q_1} ||| S_q \rangle\rangle_{3\omega,2\omega,\omega} \quad (36)$$

利用(36)式，和$\delta_{gf_2} = \frac{1}{N}\sum_{q_2} e^{i(g-f_2,q_2)}$；

$$J(q+q_1+q_2) = \sum_{f_3} J_{gf_3} e^{i(f_3-g,q+q_1+q_2)}$$

(35)式变为

$$\left.\begin{aligned}
&3\omega\langle\langle S^x_{-q-q_1q_2}|S^z_{q_2}||S^z_{q_1}|||S^z_q\rangle\rangle_{3\omega,2\omega,\omega}=-\frac{i}{2\pi N^{\frac{1}{2}}}\langle\langle S^y_{-q-q_1}|S^z_{q_1}||S^z_q\rangle\rangle_{2\omega,\omega}\\
&\qquad+iSJ_0\langle\langle S^z_{-q-q_1-q_2}|S^z_{q_2}||S^z_{q_1}|||S^z_q\rangle\rangle_{3\omega,2\omega,\omega}\\
&3\omega\langle\langle S^y_{-q-q_1-q_2}|S^z_{q_2}||S^z_{q_1}|||S^z_q\rangle\rangle_{3\omega,2\omega,\omega}=\frac{i}{2\pi N^{\frac{1}{2}}}\langle\langle S^x_{-q-q_1}|S^z_{q_1}||S^z_q\rangle\rangle_{2\omega,\omega}\\
&\qquad+i\Omega\langle\langle S^z_{-q-q_1-q_2}|S^z_{q_2}||S^z_{q_1}|||S^z_q\rangle\rangle_{3\omega,2\omega,\omega}\\
&\qquad-iSJ_0\langle\langle S^x_{-q-q_1-q_2}|S^z_{q_2}||S^z_{q_1}|||S^z_q\rangle\rangle_{3\omega,2\omega,\omega}\\
&\qquad-ixJ(q+q_1+q_2)\langle\langle S^z_{-q-q_1-q_2}|S^z_{q_2}||S^z_{q_1}|||S^z_q\rangle\rangle_{3\omega,2\omega,\omega}\\
&3\omega\langle\langle S^z_{-q-q_1-q_2}|S^z_{q_2}||S^z_{q_1}|||S^z_q\rangle\rangle_{3\omega,2\omega,\omega}=-i\Omega\langle\langle S^y_{-q-q_1-q_2}|S^z_{q_2}||S^z_{q_1}|||S^z_q\rangle\rangle_{3\omega,2\omega,\omega}
\end{aligned}\right\}\quad(37)$$

由(37)式可解出。

$$\langle\langle S^z_{-q-q_1-q_2}|S^z_{q_2}||S^z_q|||S^z_{q_1}\rangle\rangle_{3\omega,2\omega,\omega}$$

$$=\frac{x\Omega\{(2\omega)^2+4S^2J_0^2-\Omega[\Omega-xJ(q+q_1+q_2)]\}}{2(2\pi)^3N(\omega^2-\omega_q^2)\left[(2\omega)^2-\omega^2_{q+q_1}\right]\left[(3\omega)^2-\omega^2_{q+q_1+q_2}\right]}\quad(38)$$

将(36)(38)式代入(33)式可得三倍频的极化强度与外电场的关系为

$$\delta^{(3)}\langle P_z(t)\rangle=-\mu^4N_0(2\pi)^3N\langle\langle S_0^z|S_0^z||S_0^z|||S_0^z\rangle\rangle_{3\omega,2\omega,\omega}E_z^3(e^{-i3\omega t}+e^{i3\omega t})$$

$$=-\frac{\mu^4N_0x\{(2\omega)^2+4S^2J_0^2-\Omega(\Omega-xJ_0)\}E_z^3}{2(\omega^2-\omega_0^2)\left[(2\omega)^2-\omega_0^2\right]\left[(3\omega)^2-\omega_0^2\right]}(e^{-i3\omega t}+e^{i3\omega t})\quad(39)$$

(39)式表明一般情况下三倍频效应比二倍频效应弱，只当$3\omega\approx\omega_0$时，三倍效应比二倍频效应强。与二倍频效应不同的是在顺电相仍可以出现三倍频效应。

四、结　论

1．从以上分析可得到用横场易兴模型来描写的铁电晶体具有如下的性质：

①极化过程的线性效应：系统的铁电共振频率为ω_0，ω_0就是软模频率，当外极化场的频率ω等于ω_0时线性极化率达到极大。另外，当温度到达铁电转变温度时静态线性极化率趋于无穷大。

②极化过程的非线性效应：系统具有倍频、检波、混频等一系列非线性效应。当$2\omega\cong\omega_0$时二倍频效应最强，当$3\omega\cong\omega_0$时三倍频效应最强，对二倍频效应，只当系统处于铁电相时(即系统为非中心对称时)才能发生，自发极化越大隧道积分越大二倍频效应越强。

2。利用系统是否存在极化过程的非线性效应可以判断该系统是属于有序—无序型铁电性或者位移型铁电性。

3。利用铁电共振和非线性效应有可能用铁电体制成远红外波段的器件,如检波器,讯号发生器，放大器，调制器等，这类型的器件能否实现有待进一步的研究。

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The Non-linear Effects of the Ising Model in a Transverse Field

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Abstract

In this paper, we applied the method of the n+1 time Green function to analyse the linear and non-linear effects of the longitudinal polarization process of the ising model in a transvers field. The linear and non-linear polarizab- ilities and detection, mixing frequency, munltiplying frequency, effects was obtained The relations between these effects and the tunnelling integration, the interaction integration, the frequency, the temperature was explained.