

介观电容耦合 LC 电路在有限温度下的能量及热效应^{*}

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由正则量子化方法导出了介观电容耦合 LC 电路体系的哈密顿算符, 利用么正变换使哈密顿算符对角化. 用系综理论给出了体系的平均能量及其涨落, 在此基础上, 借助于广义 Hellmann-Feynman 定理, 讨论了有限温度下电路体系中电荷与自感磁通的量子涨落. 结果表明, 体系中电荷与自感磁通的量子涨落不仅与电路元件参数有关, 而且还与温度有关.

关键词: 介观电路, 量子涨落, 广义 Hellmann-Feynman 定理, 有限温度

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1. 引 言

近些年来, 随着微加工技术的发展, 许多电路和器件的工艺尺寸已达到纳米量级^[1], 有关介观电路体系的量子特性也越来越受到物理学家们的关注. 早在 20 世纪 70 年代初, Louise^[2]通过与经典简谐振子量子化方法作类比实现了介观 LC 电路的量子化, 并研究了真空态下电荷和电流的量子涨落. 之后, 大量文献分别对 LC , RLC 电路^[3-7]与存在耦合的介观电路^[8-11]进行了广泛的研究. 由于实际电路一般都会产生焦耳热且工作在一定的环境温度下, 因而考虑温度对介观电路的影响就显得尤为重要. 文献[12, 13]用热场动力学理论研究了电路在有限温度下的量子效应, 文献[14-16]借助于量子算符及其 Weyl-Wigner 对应, 研究了介观电路中量子涨落受温度的影响. 本文将在推导出系综平均能量的基础上, 借助广义 Hellmann-Feynman 定理^[17]研究介观电容耦合 LC 电路体系在有限温度下电荷及自感磁通量的量子涨落.

2. 广义 Hellmann-Feynman 定理

为下面行文和完备起见, 我们先来回顾一下有关系综平均意义下的广义 Hellmann-Feynman

定理^[17].

设量子体系哈密顿算符 \hat{H} 依赖于实参数 λ , 与其本征态 $|\psi_n\rangle$ 对应的本征值为 E_n , 即 $\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$. 由 Hellmann-Feynman 定理得

$$\frac{\partial E_n}{\partial \lambda} = \langle \psi_n | \frac{\partial \hat{H}}{\partial \lambda} | \psi_n \rangle, \quad (1)$$

在热平衡混合态下, 量子体系密度算符为

$$\rho = \sum_n e^{-\beta E_n} |\psi_n\rangle \langle \psi_n|, \quad (2)$$

式中 $\beta = (kT)^{-1}$, k 为玻尔兹曼常数, T 为绝对温度. 则系综平均能量 $\langle \hat{H}(\lambda) \rangle_e$ 可表示为

$$\begin{aligned} \langle \hat{H}(\lambda) \rangle_e &= \frac{\text{Tr}(\rho \hat{H}(\lambda))}{Z(\lambda)} \\ &= \frac{1}{Z(\lambda)} \sum_n e^{-\beta E_n(\lambda)} E_n(\lambda) \\ &= \bar{E}(\lambda), \end{aligned} \quad (3)$$

式中, $Z = \text{Tr} \rho$ 为配分函数, 下标 e 表示系综平均. 将(3)式对参量 λ 求偏微分得

$$\begin{aligned} \frac{\partial \bar{E}(\lambda)}{\partial \lambda} &= \frac{1}{Z^2(\lambda)} \left\{ Z(\lambda) \sum_n e^{-\beta E_n(\lambda)} \right. \\ &\quad \times [-\beta E_n(\lambda) + 1] \frac{\partial E_n(\lambda)}{\partial \lambda} \\ &\quad \left. - \left[\sum_n e^{-\beta E_n(\lambda)} E_n(\lambda) \right] \right. \\ &\quad \left. \times \left[\sum_n e^{-\beta E_n(\lambda)} \frac{\partial E_n(\lambda)}{\partial \lambda} \right] \{-\beta\} \right\} \end{aligned}$$

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$$= \frac{1}{Z(\lambda)} \left\{ \sum_n e^{-\beta E_n(\lambda)} \left[-\beta E_n(\lambda) + \beta \bar{E}(\lambda) + 1 \right] \frac{\partial E_n(\lambda)}{\partial \lambda} \right\}, \quad (4)$$

将(1)式代入(4)式得

$$\begin{aligned} \frac{\partial \hat{H}(\lambda)_e}{\partial \lambda} &= \frac{\partial \bar{E}(\lambda)}{\partial \lambda} \\ &= [1 + \beta \bar{E}(\lambda) - \beta \hat{H}(\lambda)] \frac{\partial \hat{H}(\lambda)_e}{\partial \lambda}. \end{aligned} \quad (5)$$

此即系综平均意义下的广义 Hellmann-Feynman 定理^[17]. 当体系哈密顿 \hat{H} 与 β 无关时, 可将上式简化为

$$\begin{aligned} \frac{\partial \bar{E}(\lambda)}{\partial \lambda} &= [1 + \beta \bar{E}(\lambda)] \frac{\partial \hat{H}(\lambda)_e}{\partial \lambda} - \beta \left[-\frac{\partial}{\partial \beta} \frac{\partial \hat{H}(\lambda)_e}{\partial \lambda} + \frac{\partial \hat{H}(\lambda)_e}{\partial \lambda} \bar{E}(\lambda) \right] \\ &= \frac{\partial}{\partial \beta} \left[\beta \frac{\partial \hat{H}(\lambda)_e}{\partial \lambda} \right]. \end{aligned} \quad (6)$$

3. 介观电容耦合 LC 电路的量子化

对于如图 1 所示的介观电容耦合 LC 电路, C_i ($i=1, 2$) 表示第 i 个支路中的电容, L_i ($i=1, 2$) 表示第 i 个支路中的电感, C_c 为耦合电容.

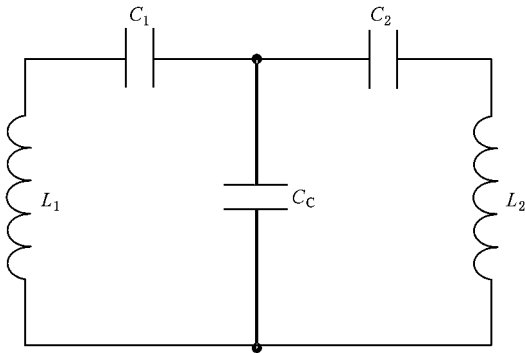


图 1 介观电容耦合 LC 电路示意图

假设电路被瞬时脉冲所激发, 如果把支路中的电荷 q_i ($i=1, 2$) 视为广义坐标, 则体系的广义势能为

$$V = \frac{1}{2C_1} q_1^2 + \frac{1}{2C_2} q_2^2 + \frac{1}{2C_c} (q_1 - q_2)^2, \quad (7)$$

相应地, 体系的广义动能为

$$T = \frac{1}{2} L_1 \dot{q}_1^2 + \frac{1}{2} L_2 \dot{q}_2^2. \quad (8)$$

于是, 对应体系的拉格朗日函数可写成为

$$l = T - V = \frac{1}{2} L_1 \dot{q}_1^2 + \frac{1}{2} L_2 \dot{q}_2^2 - \frac{1}{2C_1} q_1^2 - \frac{1}{2C_2} q_2^2 - \frac{1}{2C_c} (q_1 - q_2)^2. \quad (9)$$

由(9)式可以得到与 q_1 和 q_2 共轭的广义动量分别为

$$\begin{aligned} p_1 &= \frac{\partial l}{\partial \dot{q}_1} = L_1 \dot{q}_1, \\ p_2 &= \frac{\partial l}{\partial \dot{q}_2} = L_2 \dot{q}_2. \end{aligned} \quad (10)$$

由上式可知, p_1 和 p_2 分别为两回路中的自感磁通量, 除因子 L_1 和 L_2 外反映了电流的大小. 结合(9)式和(10)式可得电路体系的哈密顿量为

$$\begin{aligned} H &= \sum_{i=1}^2 p_i \dot{q}_i - l \\ &= \frac{1}{2} \sum_{i=1}^2 \left[\frac{p_i^2}{L_i} + \left(\frac{1}{C_i} + \frac{1}{C_c} \right) q_i^2 \right] - \frac{q_1 q_2}{C_c}, \end{aligned} \quad (11)$$

由标准的正则量子化方法^[18]可知, 一对正则共轭变量 q_i 和 p_i 与一对厄米算符 \hat{q}_i 和 \hat{p}_i 相对应, 它们之间满足对易关系 $[\hat{q}_i, \hat{p}_i] = i\hbar$. 故量子化后体系的哈密顿算符可写成为

$$\hat{H} = \frac{1}{2} \sum_{i=1}^2 \left[\frac{\hat{p}_i^2}{L_i} + \left(\frac{1}{C_i} + \frac{1}{C_c} \right) \hat{q}_i^2 \right] - \frac{\hat{q}_1 \hat{q}_2}{C_c}. \quad (12)$$

为使其对角化, 引入下面的幺正变换^[19, 20]:

$$\hat{U} = \int_{-\infty}^{+\infty} dq_1 dq_2 \left| \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \right|, \quad (13)$$

式中 A, B, C 和 D 皆为实数, 且满足 $AD - BC = 1$.

$\left| \begin{pmatrix} q_1 \\ q_2 \end{pmatrix} \right\rangle = |q_1, q_2\rangle$, $|q_i\rangle$ 为坐标本征态, 它在 Fock 表象中表示为

$$\begin{aligned} |q_i\rangle &= \left(\frac{m_i \omega_i}{\pi \hbar} \right)^{1/4} \exp \left\{ -\frac{m_i \omega_i}{2\hbar} q_i^2 + \sqrt{\frac{2m_i \omega_i}{\hbar}} q_i \hat{a}_i^\dagger - \frac{\hat{a}_i^{\dagger 2}}{2} \right\} |0\rangle, \end{aligned} \quad (14)$$

这里选取

$$A = (L_2/L_1)^{1/4} \cos \frac{\varphi}{2},$$

$$B = -(L_2/L_1)^{1/4} \sin \frac{\varphi}{2},$$

$$C = (L_1/L_2)^{1/4} \sin \frac{\varphi}{2},$$

$$D = (L_1/L_2)^{1/4} \cos \frac{\varphi}{2},$$

$$\tan \varphi = \frac{2C_1 C_2 \sqrt{L_1 L_2}}{L_1 C_1 (C_c + C_2) - L_2 C_2 (C_c + C_1)} \quad (15)$$

利用么正算符 \hat{U} 可得^[20]

$$\begin{aligned} \hat{U}^{-1} \hat{q}_1 \hat{U} &= A \hat{q}_1 + B \hat{q}_2, \\ \hat{U}^{-1} \hat{q}_2 \hat{U} &= C \hat{q}_1 + D \hat{q}_2, \\ \hat{U}^{-1} \hat{p}_1 \hat{U} &= D \hat{p}_1 - C \hat{p}_2, \\ \hat{U}^{-1} \hat{p}_2 \hat{U} &= -B \hat{p}_1 + A \hat{p}_2. \end{aligned} \quad (16)$$

由(16)式可得出么正变换后的哈密顿算符为

$$\begin{aligned} \hat{H}' &= \hat{U}^{-1} \hat{H} \hat{U} = \frac{\hat{p}_1^2}{2m_1} + \frac{\hat{p}_2^2}{2m_2} \\ &+ \frac{1}{2} m_1 \omega_1^2 \hat{q}_1^2 + \frac{1}{2} m_2 \omega_2^2 \hat{q}_2^2, \end{aligned} \quad (17)$$

式中

$$\begin{aligned} m_1 &= m_2 = \sqrt{L_1 L_2}, \\ \omega_1^2 &= \frac{1}{\sqrt{L_1 L_2}} \left[\left(\frac{1}{C_1} + \frac{1}{C_c} \right) A^2 + \left(\frac{1}{C_2} + \frac{1}{C_c} \right) C^2 - \frac{2AC}{C_c} \right], \\ \omega_2^2 &= \frac{1}{\sqrt{L_1 L_2}} \left[\left(\frac{1}{C_1} + \frac{1}{C_c} \right) B^2 + \left(\frac{1}{C_2} + \frac{1}{C_c} \right) D^2 - \frac{2BD}{C_c} \right]. \end{aligned} \quad (18)$$

可见,体系的哈密顿算符经过么正变换后可等效为两独立的量子力学简谐振子的哈密顿算符. 其中 m_1 和 m_2 分别为两个简谐振子的广义质量, ω_1 和 ω_2 为对应简谐振子的振动频率. 由 $[\hat{q}_i, \hat{p}_i] = i\hbar$, 可构造出如下的玻色子算符:

$$\begin{aligned} \hat{a}_i &= \sqrt{\frac{m_i \omega_i}{2\hbar}} \left(\hat{q}_i + \frac{i}{m_i \omega_i} \hat{p}_i \right), \\ \hat{a}_i^\dagger &= \sqrt{\frac{m_i \omega_i}{2\hbar}} \left(\hat{q}_i - \frac{i}{m_i \omega_i} \hat{p}_i \right), \end{aligned} \quad (19)$$

且满足 $[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij}$, $[\hat{a}_i, \hat{a}_j] = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] = 0$ ($i, j = 1, 2$). 这样对角化后的体系哈密顿算符就可表示为

$$\begin{aligned} \hat{H}' &= \hbar \omega_1 \left(\hat{a}_1 \hat{a}_1^\dagger + \frac{1}{2} \right) + \hbar \omega_2 \left(\hat{a}_2 \hat{a}_2^\dagger + \frac{1}{2} \right) \\ &= \hat{H}'_1 + \hat{H}'_2. \end{aligned} \quad (20)$$

所以,相应电路体系的能级为

$$E = \sum_{i=1,2} \hbar \omega_i \left(n_i + \frac{1}{2} \right). \quad (21)$$

4. 有限温度下电路体系的能量及其涨落

由(3)式可知对角化前后系综平均能量不发生

变化,故可表示为

$$\hat{H}_e = \hat{H}'_e = \hat{H}'_{1e} + \hat{H}'_{2e}, \quad (22)$$

对于单个的简谐振子,设其哈密顿为 \hat{H}_0 ,可求出

$$\hat{H}_{0e} = \bar{E}_0 = \frac{\text{Tr}(\rho_0 \hat{H}_0)}{\text{Tr} \rho_0} = \frac{\hbar \omega_0}{2} \coth \frac{\beta \hbar \omega_0}{2}, \quad (23)$$

故电路体系有限温度下平均能量的表达式为

$$\bar{E} = \hat{H}_e = \frac{\hbar \omega_1}{2} \coth \frac{\beta \hbar \omega_1}{2} + \frac{\hbar \omega_2}{2} \coth \frac{\beta \hbar \omega_2}{2}. \quad (24)$$

若将(3)式左边对 β 求导,可以得到

$$\begin{aligned} \frac{\partial \hat{H}_e}{\partial \beta} &= - \frac{\text{Tr}(e^{-\beta \hat{H}} \hat{H}^2)}{\text{Tr}(e^{-\beta \hat{H}})} - \frac{\text{Tr}(e^{-\beta \hat{H}} \hat{H})}{[\text{Tr}(e^{-\beta \hat{H}})]^2} \text{Tr}(e^{-\beta \hat{H}}) \\ &= - \frac{\text{Tr}(e^{-\beta \hat{H}} \hat{H}^2) - \bar{E}^2 \text{Tr}(e^{-\beta \hat{H}})}{\text{Tr}(e^{-\beta \hat{H}})} \\ &= - \hat{H}^2 - \bar{E}^2_e = -(\Delta \hat{H})^2, \end{aligned} \quad (25)$$

所以在有限温度下能量的量子涨落为

$$\begin{aligned} (\Delta \hat{H})^2 &= - \frac{\partial \hat{H}_e}{\partial \beta} = \frac{\hbar^2 \omega_1^2}{4} \frac{1}{\sinh^2 \frac{\beta \hbar \omega_1}{2}} \\ &+ \frac{\hbar^2 \omega_2^2}{4} \frac{1}{\sinh^2 \frac{\beta \hbar \omega_2}{2}}. \end{aligned} \quad (26)$$

结合双曲余切和双曲正弦函数的性质分析(24)和(26)式,可以知道在有限温度下平均能量 \bar{E} 和其量子涨落 $(\Delta \hat{H})^2$ 都随着温度的升高而变大.

5. 有限温度下回路体系中电荷与自感磁通量的量子涨落

由文献[17]知道,应用广义 Hellmann-Feynman 定理可以求出哈密顿量中一些变量在有限温度下的量子涨落,据此,可得到回路体系中电荷与自感磁通量的量子涨落.

因体系哈密顿 \hat{H} 与 β 无关,若将(6)式两边同时对参量 β 积分,则有

$$\beta \frac{\partial \hat{H}(\lambda)}{\partial \lambda} = \int d\beta \frac{\partial}{\partial \lambda} \bar{E}(\lambda), \quad (27)$$

如果取 $\lambda_1 = 1/L_1$,将(12)和(24)式代入上式可得出

$$\beta \frac{\partial \hat{H}}{\partial (1/L_1)} = \beta \frac{1}{2} \hat{p}_1^2 = \int d\beta \frac{\partial}{\partial (1/L_1)} \bar{E}, \quad (28)$$

即可得到 \hat{p}_1^2 的具体形式为

$$\begin{aligned} \hat{p}_{1e}^2 &= \hbar \left[\frac{\partial \omega_1}{\partial (1/L_1)} \coth \frac{\beta \hbar \omega_1}{2} + \frac{\partial \omega_2}{\partial (1/L_1)} \coth \frac{\beta \hbar \omega_2}{2} \right] \\ &= \frac{\hbar}{2} \left(\frac{1}{C_1} + \frac{1}{C_c} \right) \left[\frac{1}{\omega_1} \coth \left(\frac{\beta \hbar \omega_1}{2} \right) \cos^2 \frac{\varphi}{2} \right. \\ &\quad \left. + \frac{1}{\omega_2} \coth \left(\frac{\beta \hbar \omega_2}{2} \right) \sin^2 \frac{\varphi}{2} \right]. \end{aligned} \quad (29)$$

同理若分别取 $\lambda_2 = 1/L_2$, $\lambda_3 = 1/C_1 + 1/C_c$, $\lambda_4 = 1/C_2 + 1/C_c$, 即可分别得到

$$\begin{aligned} \hat{p}_{2e}^2 &= \frac{\hbar}{2} \left(\frac{1}{C_2} + \frac{1}{C_c} \right) \left[\frac{1}{\omega_1} \coth \left(\frac{\beta \hbar \omega_1}{2} \right) \sin^2 \frac{\varphi}{2} \right. \\ &\quad \left. + \frac{1}{\omega_2} \coth \left(\frac{\beta \hbar \omega_2}{2} \right) \cos^2 \frac{\varphi}{2} \right], \end{aligned} \quad (30)$$

$$\begin{aligned} \hat{q}_{1e}^2 &= \frac{\hbar}{2L_1} \left[\frac{1}{\omega_1} \coth \left(\frac{\beta \hbar \omega_1}{2} \right) \cos^2 \frac{\varphi}{2} \right. \\ &\quad \left. + \frac{1}{\omega_2} \coth \left(\frac{\beta \hbar \omega_2}{2} \right) \sin^2 \frac{\varphi}{2} \right], \end{aligned} \quad (31)$$

$$\begin{aligned} \hat{q}_{2e}^2 &= \frac{\hbar}{2L_2} \left[\frac{1}{\omega_1} \coth \left(\frac{\beta \hbar \omega_1}{2} \right) \sin^2 \frac{\varphi}{2} \right. \\ &\quad \left. + \frac{1}{\omega_2} \coth \left(\frac{\beta \hbar \omega_2}{2} \right) \cos^2 \frac{\varphi}{2} \right]. \end{aligned} \quad (32)$$

由于 $\hat{q}_{ie} = \hat{p}_{ie} = \alpha (i = 1, 2)$, 所以电路体系中电荷与自感磁通量的量子涨落分别为

$$\begin{aligned} (\Delta \hat{p}_1)^2 &= \frac{\hbar}{2} \left(\frac{1}{C_1} + \frac{1}{C_c} \right) \left[\frac{1}{\omega_1} \coth \left(\frac{\beta \hbar \omega_1}{2} \right) \cos^2 \frac{\varphi}{2} \right. \\ &\quad \left. + \frac{1}{\omega_2} \coth \left(\frac{\beta \hbar \omega_2}{2} \right) \sin^2 \frac{\varphi}{2} \right], \end{aligned} \quad (33)$$

$$\begin{aligned} (\Delta \hat{p}_2)^2 &= \frac{\hbar}{2} \left(\frac{1}{C_2} + \frac{1}{C_c} \right) \left[\frac{1}{\omega_1} \coth \left(\frac{\beta \hbar \omega_1}{2} \right) \sin^2 \frac{\varphi}{2} \right. \\ &\quad \left. + \frac{1}{\omega_2} \coth \left(\frac{\beta \hbar \omega_2}{2} \right) \cos^2 \frac{\varphi}{2} \right], \end{aligned} \quad (34)$$

$$\begin{aligned} (\Delta \hat{q}_1)^2 &= \frac{\hbar}{2L_1} \left[\frac{1}{\omega_1} \coth \left(\frac{\beta \hbar \omega_1}{2} \right) \cos^2 \frac{\varphi}{2} \right. \\ &\quad \left. + \frac{1}{\omega_2} \coth \left(\frac{\beta \hbar \omega_2}{2} \right) \sin^2 \frac{\varphi}{2} \right], \end{aligned} \quad (35)$$

$$\begin{aligned} (\Delta \hat{q}_2)^2 &= \frac{\hbar}{2L_2} \left[\frac{1}{\omega_1} \coth \left(\frac{\beta \hbar \omega_1}{2} \right) \sin^2 \frac{\varphi}{2} \right. \\ &\quad \left. + \frac{1}{\omega_2} \coth \left(\frac{\beta \hbar \omega_2}{2} \right) \cos^2 \frac{\varphi}{2} \right]. \end{aligned} \quad (36)$$

注意到 $T > 0$ K 时, $\coth(\beta \hbar \omega_i / 2)$ ($i = 1, 2$) 为恒大于 1 的单调增函数, 由(33)–(36)式可知: 当电路元件参数确定后, 由于电流在电路中运动会产生焦耳热, 以及受环境温度的影响, 电路体系中电荷与回路自感磁通量的量子涨落都随着温度的升高而单调地增加. 当温度很低时, $\coth(\beta \hbar \omega_i / 2) \rightarrow 1$, 回路中的电荷与自感磁通量的涨落均显含普朗克常量, 此时, 量子噪声起主要作用; 当温度很高时, $\coth(\beta \hbar \omega_i / 2) \rightarrow 2k(\beta \hbar \omega_i)$, 这使普朗克常量从涨落中消失, 此时, 经典噪声起主要作用. 通过验证, 还可以得到 \hat{q}_i 和 \hat{p}_i 满足的不确定关系为 $(\Delta \hat{q}_i)^2 (\Delta \hat{p}_i)^2 \geq \hbar^2 / 4$.

6. 结 论

对于本文所讨论的介观电容耦合 LC 电路, 从拉格朗日函数出发, 将回路中的电荷作为广义坐标, 用正则量子化方法导出其电路体系的哈密顿算符. 通过引入么正算符实现了体系哈密顿算符的对角化. 在此基础上, 研究了热平衡混态中电路体系的系综平均能量, 以及该能量在温度影响下的量子涨落, 并借助于广义 Hellmann-Feynman 定理, 讨论了回路中电荷算符及自感磁通算符的量子涨落. 结果表明, 电路体系的电荷算符及自感磁通算符的量子涨落不仅与电路中各元件参量有关系, 而且还与温度密切相关, 二者随着温度的升高, 都有所增加. 所以, 在实际微型电路的设计中, 除了要考虑各元件参量之外, 还需考虑环境温度的影响, 这对于设计低噪声的微型电路有一定的指导意义.

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The energy and thermal effects of mesoscopic capacitance coupling LC circuit at finite temperature^{*}

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Abstract

For the mesoscopic capacitance coupling LC circuit , the Hamiltonian is given by the canonical quantization. The Hamiltonian operator is diagonalized by a unitary transformation. The ensemble average energy and its fluctuations are derived by ensemble theory. In virtue of the generalized Hellmann-Feynman theorem , the quantum fluctuations of charge and self-conductance magnetic flux for the system at finite temperature are investigated. It is found that , the quantum fluctuations of charge and self-conductance magnetic flux depend on the temperature as well as the parameters of the circuit components.

Keywords : mesoscopic circuit , quantum fluctuation , generalized Hellmann-Feynman theorem , finite temperature

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