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有限温度下多维裂变速率的量子修正*

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摘　　要

用路径积分方法得到了有限温度下多维量子裂变速率的表达式.

量子 Kramers 问题是通过引入关于集体坐标、环境谐振子及其两者之间的耦合的总 Lagrangian 量来描述的[1]. 最近的工作是基于路径积分技巧,在准经典 WKB 近似下,考虑了一个伸长自由度,并通过计算自由能虚部得到了量子裂变速率公式[2,3]. 本文旨在导出跨越温度以上的多维裂变速率的量子修正项. 在这样宽的温度区域内加入量子涨落效应后,热翻越机制仍对裂变起主要作用.

我们所关心的模型 Lagrangian 量为

$$L = \sum_{i,j=1}^{N} \frac{1}{2} M_{ij}\dot{R}_i\dot{R}_j - V(R_1, R_2, \cdots, R_N) + \sum_{\alpha=1}^{I} \frac{m_\alpha}{2} (\dot{q}_\alpha^2 - \omega_\alpha^2 q_\alpha^2)$$

$$- \sum_{\alpha=1}^{I} q_\alpha f_\alpha(R_1, R_2, \cdots, R_N), \tag{1}$$

式中 $N \ll I$, R_i 和 q_α 分别是裂变和环境振子坐标,最后一项代表其间的非线性耦合.

从方程(1),我们获得经典运动方程

$$\sum_{j=1}^{N} M_{ij}\ddot{R}_j = -\frac{\partial V}{\partial R_i} - \sum_{\alpha=1}^{I} q_\alpha \frac{\partial}{\partial R_i} f_\alpha(R_1, R_2, \cdots, R_N), \tag{2}$$

$$m_\alpha \ddot{q}_\alpha = -m_\alpha \omega_0^2 q_\alpha - f_\alpha(R_1, R_2, \cdots, R_N). \tag{3}$$

为在方程(2)中消去内禀坐标,可将方程(3)的一般解

$$q_\alpha(t) = q_\alpha(0)\cos\omega_\alpha t + \frac{\dot{q}_\alpha(0)}{\omega_\alpha}\sin\omega_\alpha t - \int_0^t ds\, \frac{\sin[\omega_\alpha(t-s)]}{m_\alpha\omega_\alpha}$$

$$\times f_\alpha(R_1, R_2, \cdots, R_N), \tag{4}$$

代入. 完成分部积分后,给出广义 Langevin 方程

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$$\sum_{j=1}^{N} M_{ij}\ddot{R}_j = -\frac{\partial V_{eff}}{\partial R_i} - \int_0^t \sum_{j=1}^{N} \nu_{ij}(t,s)\dot{R}_j(s)\mathrm{d}s + \xi_i(t), \tag{5}$$

这里重整化势,阻尼张量和无规力分别为

$$V_{eff} = V(R_1,R_2,\cdots,R_N) - \sum_{\alpha=1}^{I} \frac{1}{2m_\alpha\omega_\alpha^2} f_\alpha^2(R_1, R_2,\cdots,R_N), \tag{6}$$

$$\nu_{ij}(t, s) = \sum_{\alpha=1}^{I} \frac{\cos[\omega_\alpha(t-s)]}{m_\alpha\omega_\alpha^2} \cdot \frac{\partial f_\alpha[R_1(t),R_2(t),\cdots, R_N(t)]}{\partial R_i} \cdot \frac{\partial f_\alpha[R_1(s), R_2(s),\cdots,R_N(s)]}{\partial R_j}, \tag{7}$$

和

$$\xi_i(t) = -\sum_{\alpha=1}^{I}\left[\left(q_\alpha(0) + \frac{f_\alpha(R(0))}{m_\alpha\omega_\alpha^2}\right)\cos\omega_\alpha t + \frac{\dot{q}_\alpha(0)}{\omega_\alpha}\sin\omega_\alpha t\right]\frac{\partial f_\alpha(R(t))}{\partial R_i}. \tag{8}$$

N维裂变核系统在温度 $k_B T = \frac{1}{\beta}$ 的配分函数的路径积分表述是

$$Z(\beta) = \int \mathscr{D}[R_1]\mathscr{D}[R_2]\cdots\mathscr{D}[R_N]\exp[-S_{eff}(R_1,R_2,\cdots,R_N)/\hbar]. \tag{9}$$

二阶有效作用量写作

$$S_{eff}(R_1,R_2,\cdots,R_N) = \int_0^{\hbar\beta}\mathrm{d}\tau\left[\sum_{i,j=1}^{N}\frac{1}{2}M_{ij}\dot{R}_i\dot{R}_j + V_{eff}(R_1,R_2,\cdots,R_N)\right] + \frac{1}{2}\int_0^{\hbar\beta}\mathrm{d}\tau\int_0^{\hbar\beta}\mathrm{d}\tau'\sum_{i,j=1}^{N}k_{ij}(\tau-\tau')R_i(\tau)R_j(\tau'), \tag{10}$$

式中影响函数为

$$k_{ij}(\tau-\tau') = \sum_{\alpha=1}^{I}\left[\frac{1}{m_\alpha\omega_\alpha^2}:\delta(\tau-\tau'): - \frac{\cosh\left[\omega_\alpha\left(|\tau-\tau'| - \frac{\hbar\beta}{2}\right)\right]}{2m_\alpha\omega_\alpha\sinh\left(\frac{1}{2}\hbar\beta\omega_\alpha\right)}\right] \cdot \frac{\partial f_\alpha(R)}{\partial R_i}\cdot\frac{\partial f_\alpha(R)}{\partial R_j}, \tag{11}$$

这里:$\delta(\tau-\tau')$:是一个以 $\hbar\beta$ 为周期的广义 δ 函数[2]. 推导中，将基态和鞍点的惯性质量处理为两个相异的常数矩阵，而耦合函数 $f_\alpha(\mathbf{R})$已在这两处泰勒展开到一级. 阻尼核函数 $k_{ij}(\tau)$ 可以展开成 Fourier 级数和

$$k_{ij}(\tau) = \frac{1}{\hbar\beta}\sum_{n=-\infty}^{\infty}K_{ij}(\theta_n)\exp(i\theta_n\tau), \tag{12}$$

式中 $\theta_n = 2\pi n/\hbar\beta$ 是环境玻色子的 Matsubare 频率. 与频率有关的 Fourier 系数可由阻尼核函数(7)的 Laplace 变换给出

$$K_{ij}(\theta_n) = |\theta_n|\hat{\nu}_{ij}(|\theta_n|), \tag{13}$$

而

$$\hat{\nu}_{ij}(|\theta_n|) = \sum_{\alpha=1}^{I}\left[\frac{|\theta_n|}{m_\alpha\omega_\alpha^2(\theta_n^2+\omega_\alpha^2)}\cdot\frac{\partial f_\alpha}{\partial R_i}\cdot\frac{\partial f_\alpha}{\partial R_j}\right]. \tag{14}$$

在基态,有效形变势能近似写成

$$V_{\rm eff}(R_1, R_2, \cdots, R_N) = \sum_{i,j=1}^{N} \frac{1}{2} W_{ij}^{\rm eff}(R_i - R_i^0)(R_j - R_j^0) - V_b^{\rm eff}. \tag{15}$$

依照准经典近似,对泛函积分(9)式起主要贡献的来自稳定路径附近的扰动项,它们可以表作如下周期轨道的形式

$$R_i^0(\tau) = \sum_{n=-\infty}^{\infty} X_n^i \exp(i\theta_{n0}\tau). \tag{16}$$

则

$$\begin{aligned} Z_0(\beta) &= J_1 \exp(\beta_0 V_b^{\rm eff}) \int \prod_{i=1}^{N} \prod_{n=-\infty}^{\infty} \mathscr{D}[X_n^i] \exp\left\{-\frac{\beta_0}{2} \sum_{n=-\infty}^{\infty} \sum_{i,j=1}^{N} [\theta_{n0}^2 M_{ij} \right. \\ &\qquad \left. + W_{ij}^{\rm eff} + |\theta_{n0}| \hat{\nu}_{ij}(|\theta_{n0}|)] X_n^i X_{-n}^j \right\} \\ &= J_2 \exp(\beta_0 V_b^{\rm eff}) \left(\frac{2\pi}{\beta_0}\right)^{\frac{N}{2}} \Big/ \sqrt{\det W_{\rm eff}} \cdot \left[\int \prod_{i=1}^{N} \prod_{n=1}^{\infty} \mathscr{D}[X_n^i] \exp\left\{-\frac{\beta_0}{2}\right.\right. \\ &\qquad \left.\left. \cdot \sum_{n=1}^{\infty} \sum_{i,j=1}^{N} (\theta_{n0}^2 M_{ij} + W_{ij}^{\rm eff} + \theta_{n0}\hat{\nu}_{ij}) X_n^i X_n^j \right\}\right]^2. \end{aligned} \tag{17}$$

考虑到惯性张量 M_{ij} 的正定性,可引入变量线性代换:

$$X_n^i = \sqrt{\frac{2\pi}{\beta_0}} \frac{1}{\theta_{n0}} \sum_{k=1}^{N} (M^{-\frac{1}{2}})_{ik} Y_n^k. \tag{18}$$

则

$$\begin{aligned} Z_0(\beta) &= J_3 \exp(\beta_0 V_b^{\rm eff}) \left(\frac{2\pi}{\beta_0}\right)^{\frac{N}{2}} \Big/ \sqrt{\det W_{\rm eff}} \left[\int \prod_{i=1}^{N} \prod_{n=1}^{\infty} \mathscr{D}[Y_n^i] \exp\left\{-\pi \right.\right. \\ &\qquad \cdot \sum_{n=1}^{\infty} \sum_{i,j=1}^{N} \left[\delta_{ij} + \frac{1}{\theta_{n0}^2} \sum_{k,l=1}^{N} (M^{-\frac{1}{2}})_{ik} W_{kl}^{\rm eff} (M^{-\frac{1}{2}})_{lj} \right. \\ &\qquad \left.\left.\left. + \frac{1}{\theta_{n0}} \sum_{k,l=1}^{N} (M^{-\frac{1}{2}})_{ik} \hat{\nu}_{kl} (M^{-\frac{1}{2}})_{lj} \right] Y_n^i Y_n^j \right\}\right]^2. \end{aligned} \tag{19}$$

若 $\hat{\nu}_{ij}$ 和 $V_b^{\rm eff}$ 等于零,上式应成为 N 维简正谐振子的配分函数,即有

$$\begin{aligned} Z_0(\beta) &= J_3 \left(\frac{2\pi}{\beta_0}\right)^{\frac{N}{2}} \Big/ \sqrt{\det W_{\rm eff}} \prod_{i=1}^{N} \prod_{n=1}^{\infty} \frac{1}{1 + \frac{\hbar^2 \beta_0^2 \omega_i^2}{4\pi^2 n^2}} \\ &= J_3 \left(\frac{2\pi}{\beta_0}\right)^{\frac{N}{2}} \Big/ \sqrt{\det W_{\rm eff}} (\hbar\beta_0)^N (\det M_0^{-1} \cdot \det W_{\rm eff})^{\frac{1}{2}} \\ &\qquad \cdot \prod_{i=1}^{N} \left[2\sinh\left(\frac{\hbar\beta_0\omega_i}{2}\right)\right]^{-1} \\ &= \prod_{i=1}^{N} \left[2\sinh\left(\frac{\hbar\beta_0\omega_i}{2}\right)\right]^{-1}, \end{aligned} \tag{20}$$

式中 ω_i 为 $M_0^{-\frac{1}{2}} W_{\rm eff} M_0^{-\frac{1}{2}}$ 的本征值,由此定出变换系数

$$J_3 = (2\pi\hbar^2\beta_0)^{-\frac{N}{2}} (\det M_0)^{\frac{1}{2}}. \tag{21}$$

脚标 0 和 s 用来表示基态和鞍点处的值．故

$$Z_0(\beta) = (\hbar\beta_0)^{-N}(\det M_0/\det W_{eff})^{\frac{1}{2}}\exp(\beta_0 V_b^{eff}) \cdot \prod_{n=1}^{\infty}\det\left(1+\frac{1}{\theta_{n0}^2}\widetilde{W}_{eff}+\frac{1}{\theta_{n0}}\tilde{\nu}_0\right)^{-1}. \tag{22}$$

这里 $\widetilde{W}_{eff} = M_0^{-\frac{1}{2}}W_{eff}M_0^{-\frac{1}{2}}$，$\tilde{\nu}_0 = M_0^{-\frac{1}{2}}\hat{\nu}_0 M_0^{-\frac{1}{2}}$。

有效形变势能在鞍点附近被写成

$$V_{eff}(R_1, R_2, \cdots, R_N) = \sum_{i,j=1}^{N}\frac{1}{2}V_{ij}^{eff}(R_i - R_i^s)(R_j - R_j^s), \tag{23}$$

它有一个负根和 $N-1$ 个正根的本征值，那么二阶有效作用量沿着不稳定方向达不到极小值．同时对周期轨道 $R_i^s(\tau) = \sum_{n=-\infty}^{\infty} X_n'^i \exp(i\theta_{ns}\tau)$ 中的振幅 X_0' 的泛函积分将发散．为保证配分函数从基态到鞍点的解析连续，Langer[4] 建立的聚结点理论指出，$Z_s(\beta)$ 在鞍点存在一个小指数的虚部，应对 X_0' 沿半正虚轴积分．仿照上述推导知

$$\mathrm{Im}Z_s(\beta) = \frac{1}{2}(\hbar\beta_s)^{-N}(\det M_s/|\det V_{eff}|)^{\frac{1}{2}} \cdot \prod_{n=1}^{\infty}\det\left(1+\frac{1}{\theta_{ns}^2}\widetilde{V}_{eff}+\frac{1}{\theta_{ns}}\tilde{\nu}_s\right)^{-1}. \tag{24}$$

裂变速率定义为[3]

$$\Gamma = -\frac{2}{\hbar}\frac{k_B T_c}{k_B T}\mathrm{Im}F = -\frac{2}{\hbar}k_B T_c\left(-\frac{\mathrm{Im}Z_s}{Z_0}\right), \tag{25}$$

其中跨越温度 $k_B T_c$ 由下式给出

$$\det\left(1+\frac{1}{\theta_{1s}^2}\widetilde{V}_{eff}+\frac{1}{\theta_{1s}}\tilde{\nu}_s\right) = 0$$

即

$$\det(H^2 M_s + H\hat{\nu}_s + V_{eff}) = 0, \tag{26}$$

式中 $H = \frac{2\pi}{\hbar}k_B T_c$。

最终得到多维量子裂变速率公式为

$$\Gamma = \frac{H}{2\pi}\left(\frac{T_s}{T_0}\right)^N\left(\frac{\det M_s \det W_{eff}}{\det M_0|\det V_{eff}|}\right)^{\frac{1}{2}}\exp(-V_b^{eff}/k_B T_0)\cdot F_q, \tag{27}$$

量子放大修正因子

$$F_q = \prod_{n=1}^{\infty}\frac{\det M_s}{\det M_0}\cdot\left[\frac{\det\left(M_0+\frac{1}{\theta_{n0}^2}\hat{\nu}_0+\frac{1}{\theta_{n0}}W_{eff}\right)}{\det\left(M_s+\frac{1}{\theta_{ns}^2}\hat{\nu}_s+\frac{1}{\theta_{ns}}V_{eff}\right)}\right]. \tag{28}$$

F_q 是个明显不小于 1 的数．这是因为量子涨落提高了亚稳态势阱中的布朗粒子的平均能量，促进它们翻越垒顶．当 T_0 和 $T_s \gg T_c$ 时，$F_q \to 1$，(27) 式自然退化为含记忆阻尼效应的非马尔科夫经典多维裂变速率的表达式[1,5]．

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Quantum Correction of the Multidimensional Fission Rate at Finite Temperature

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ABSTRACT

The expression of quantum correction of the multidimensional fission rate at finite temperature is obtained by a path integral method.