研究简报

基于辛理论的载流碳纳米管能带分析[1)]

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摘要 基于连续介质力学理论和辛弹性理论，将载流碳纳米管等效为铁木辛柯梁，采用哈密顿变分原理建立了载流碳纳米管的振动控制方程；引入对偶变量将振动控制方程从拉格朗日体系导入到哈密顿体系下；通过波传播方法分析了载流碳纳米管的能带结构；研究了流体密度、流速对载流碳纳米管能带结构的影响；同时计算了载流碳纳米管的散射矩阵. 研究发现：管内流速以及流体密度对剪切频率和弯曲频率有着非常重要的影响. 研究结果表明：载流碳纳米管的剪切频率和弯曲频率因流体的加入而减小，并随流速及流体密度的增大而减小；通过对数值结果的分析发现：载流碳纳米管由于管内流体、流速以及流体密度的作用，会使得载流碳纳米管变的更 “软”. 其中，哈密顿体系下所得出的载流碳纳米管弯曲频率随管内流体密度的增加而变小，有别于在拉格朗日体系下非局部梁理论所得的结论. 同时，数值结果表明散射矩阵是酉矩阵，辛体系下的入射波功率流与反射波功率流相等，即功率流守恒，体现了辛弹性力学理论的优越性.

关键词 碳纳米管，散射，能带，辛理论

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ANALYSING THE WAVE SCATTERING IN SINGLE-WALLED CARBON NANOTUBE CONVEYING FLUID BASED ON THE SYMPLECTIC THEORY [1)]

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Abstract Based on tcontinuum mechanics theory and the symplectic theory, the single-walled carbon nanotube (SWCNT) is modelled as a Timoshenko beam. The dynamics equations of fluid-conveying SWCNT are derived from Hamilton's principle. By introducing the symplectic variable into the mechanics system, the governing equation of fluid-conveying SWCNT is transformed from Lagrange system into Hamilton system, then the governing equation is employed to analyse the energy band structure of the SWCNT and the wave scattering in the beam. Moreover, the scattering matrix of the nanotube is calculated by symplectic methodology. The influences of the fluid density and velocity to SWCNT's band structure are also analysed. The results show that the shear and flexural frequencies of SWCNT are greater than those of fluid-conveying SWCNT. The analyses indicate that the shear and flexural frequencies of fluid-conveying SWCNT decrease with the fluid velocity and density increasing, because the effect of the fluid inside makes the nanotube softer. Meanwhile, it is also found that the scattering matrix is unitary matrix, pointing the power flow of the incident wave is equal to that of the reflected wave, indicating the power flow of Hamilton system is conserved. Furthermore, the results show the superiority of the symplectic elasticity theory.

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Key words carbon nanotube，wave scattering，energy band，symplectic theory

引 言

随着纳米科学与机械工艺的进步，纳米机电系统 (nano electro mechanical systems, NEMS) 成为当今微电子工程领域的研究热点 [1-2]. 纳米机电系统 [3] 具有尺度小、重量轻、灵敏度高、能耗低以及信息存储量大的特点. 郑泉水等 [4-5] 发现两端开口的多壁碳纳米管在范德华力驱动下会出现高频振荡. 郭万林等 [6] 在对吉赫兹量级振动器的能量耗散进行研究时发现：具有对称结构的振荡器能量耗散更大. 王琳 [7] 分析了载流管的动力学特性及稳定性. 王琳等 [8-10] 还研究了弯曲载流碳纳米管的动态响应问题. 王立峰 [11] 分别以弹性杆、壳模型和分子动力学模型，研究了碳纳米管纵波频散特性. 吉布森等 [12] 综述了有关碳纳米管的力学特性、动力学模型. Zhang 等 [13] 分析了轴向载荷下双壁碳纳米管的横向振动问题. 尹等 [14-15] 分别基于欧拉–伯努利梁理论和铁木辛柯梁理论，研究了碳纳米管波传播问题并且提出：对于太赫兹频率下的波传播分析，铁木辛柯梁理论更为准确. Wang 等 [16] 对单、双壁碳纳米管波传播特性，均做了理论及数值分析. 目前，在国际上应用非局部连续介质力学理论 [17-19] 研究碳纳米管的力学性能仍然是一个热点 [20-22].

钟万勰 [23] 将对偶体系引入到弹性力学，建立了弹性力学哈密顿系统辛求解的一般方法. 张洪武等 [22] 将应用力学辛体系应用在碳纳米管的色散关系的计算中，阐述了辛数学理论在波的界带分析上具有优势. 邓子辰 [24] 将辛数学方法应用到高频振荡系统中，而碳纳米管的特殊力学性能恰好可以实现高频振荡的需求. 因此，将辛体系应用于碳纳米管的振动分析以及波传播研究是必要的. 钟万勰 [23] 提出铁木辛柯梁的哈密顿对偶方程，并研究了铁木辛柯梁的波散射与波共振问题. 吴锋等 [25] 在此基础上，分析了铁木辛柯梁的能带结构以及波散射问题. 本文以铁木辛柯梁理论为基础，将辛弹性力学理论 [23,26] 应用于研究载流碳纳米管的波传播问题 [27-28].

1 载流碳纳米管动力学模型

本文基于铁木辛柯梁理论，应用能量变分法建立出载流碳纳米管振动分析模型 [27].

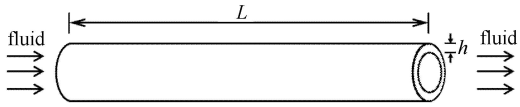


图 1 载流碳纳米管几何结构

Fig. 1 Geometry of fluid-conveying single-walled carbon nanotubes (SWCNTs)

载流碳纳米管无量纲振动控制方程 [27]

$$\left.\begin{aligned}&(1-\lambda_{\mathrm{e}})\frac{\partial^2\bar{w}}{\partial\xi^2}+\frac{\partial\bar{\phi}}{\partial\xi}-(1+\lambda_{\mathrm{d}})\frac{\partial^2\bar{w}}{\partial\eta^2}=0\\&\frac{\partial^2}{\partial\xi^2}\left[\lambda_{\mathrm{a}}+\mu(\lambda_{\mathrm{b}}+\lambda_{\mathrm{c}})\frac{\partial^2}{\partial\eta^2}\right]\bar{\phi}-(\lambda_{\mathrm{b}}+\lambda_{\mathrm{c}})\frac{\partial^2\bar{\phi}}{\partial\eta^2}-\\&\quad\left(\frac{\partial\bar{w}}{\partial\xi}+\bar{\phi}\right)=0\end{aligned}\right\}\tag{1}$$

由振动理论可知，方程 (1) 的波动解 [23] 为

$$\bar{w}(\xi,\eta)=W(\xi,\omega)\,\mathrm{e}^{-\mathrm{i}\omega\eta}\bar{\phi}(\xi,\eta)=\Phi(\xi,\omega)\,\mathrm{e}^{-\mathrm{i}\omega\eta}\tag{2}$$

其中，ω 为无量纲激励频率.

将方程 (2) 代入方程 (1)，动力学方程为

$$\left.\begin{aligned}&\frac{\mathrm{d}^2W}{\mathrm{d}\xi^2}+\frac{\mathrm{d}\Phi}{\mathrm{d}\xi}+\omega^2W+\lambda_{\mathrm{d}}\omega^2W-\lambda_{\mathrm{e}}\frac{\mathrm{d}^2W}{\mathrm{d}\xi^2}=0\\&\lambda_{\mathrm{a}}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\xi^2}-\left(\frac{\mathrm{d}W}{\mathrm{d}\xi}+\Phi\right)+(\lambda_{\mathrm{b}}+\lambda_{\mathrm{c}})\,\omega^2\Phi=0\end{aligned}\right\}\tag{3}$$

为了将拉格朗日函数导入哈密顿体系，引入对偶变量 $\boldsymbol{q}$[23]

$$\boldsymbol{p}=\frac{\partial L}{\partial\dot{\boldsymbol{q}}}=\boldsymbol{K}_{22}\dot{\boldsymbol{q}}+\boldsymbol{K}_{21}\boldsymbol{q}=\begin{bmatrix}Q_x\\-M_x\end{bmatrix}\tag{4}$$

引入向量 $\boldsymbol{v}=\begin{bmatrix}\boldsymbol{q} & \boldsymbol{p}\end{bmatrix}^{\mathrm{T}}$，方程 (3) 重新表示为 [25]

$$\dot{\boldsymbol{v}}=\boldsymbol{H}\boldsymbol{v}\tag{5}$$

2 铁木辛柯梁的能带结构

对于给定的 ω^2，位移约束

$$\dot{\boldsymbol{q}}=\mathrm{i}\mu\boldsymbol{q}\tag{6}$$

$$\left[\boldsymbol{K}_{\mathrm{qs}\mu}-\omega^2\boldsymbol{M}_{\mathrm{q}\mu}\right]\boldsymbol{q}=0\tag{7}$$

其中，μ 是波数.

$$\left.\begin{aligned}\boldsymbol{M}_{\mathrm{q}\mu} &= \begin{bmatrix} 1+\lambda_{\mathrm{d}} & 0 \\ 0 & \lambda_{\mathrm{b}}+\lambda_{\mathrm{c}} \end{bmatrix} \\ \boldsymbol{K}_{\mathrm{qs}\mu} &= \begin{bmatrix} \mu^2(1-\lambda_{\mathrm{e}}) & -\mathrm{i}\mu \\ \mathrm{i}\mu & \lambda_{\mathrm{a}}\mu^2+1 \end{bmatrix}\end{aligned}\right\} \tag{8}$$

令方程 (7) 的系数矩阵的行列式为零，这样可以得到载流碳纳米管的波传播特征方程

$$a\left(\omega^2\right)^2 + b\omega^2 + c = 0 \tag{9}$$

其中

$$\left.\begin{aligned} a &= (1+\lambda_{\mathrm{d}})(\lambda_{\mathrm{b}}+\lambda_{\mathrm{c}}) \\ b &= -\left[(1+\lambda_{\mathrm{d}})\left(\lambda_{\mathrm{a}}\mu^2+1\right) + (1-\lambda_{\mathrm{e}})(\lambda_{\mathrm{b}}+\lambda_{\mathrm{c}})\mu^2\right] \\ c &= (1-\lambda_{\mathrm{e}})\left(\lambda_{\mathrm{a}}\mu^2+1\right)\mu^2 - \mu^2 \end{aligned}\right\} \tag{10}$$

波在单壁铁木辛柯梁中的传播，只存在高频的剪切波和低频的弯曲波 [27]，相应频率分别为

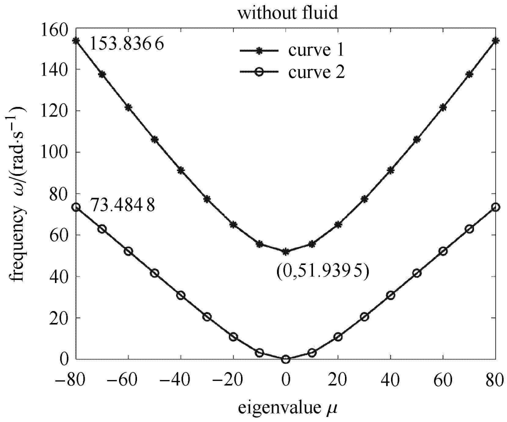
$$\omega = \sqrt{\frac{b \pm \sqrt{b^2-4ac}}{2a}} \tag{11}$$

3 数值分析与结果讨论

3.1 能带曲线

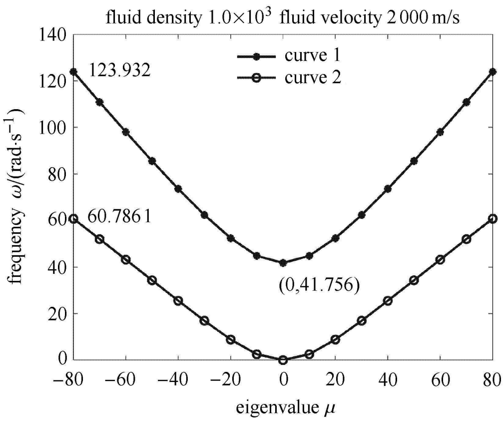
图 2 分别给出了碳纳米管无流体和有流体的能带曲线. 图 2 中，曲线 1 (Curve 1) 表示剪切波色散曲线，曲线 2 (Curve 2) 表示弯曲波色散曲线. 由图 2 不难发现：相比于无流体情况，载流碳纳米管的频率区段 $[0, \omega_{\min}]$ 变窄 (其中 $\omega_{\min}$ 为波数 μ 为零时的剪切频率，在图 2 中分别对应 51.939 5 和 41.756 0)；同时，随着碳纳米管中流体的加入，碳纳米管的弯曲频率与剪切频率均减小. 可以得到结论：由于碳纳米管内流体加入，碳纳米管会变得更 “柔软”[27]. 另外，可以发现无量纲的弯曲频率是从零开始，剪切波传播是截止频率之后开始 [28].

图 3 描述了碳纳米管能带结构随流速变化色散曲线，其中，图 3(a) 表示同一流体在不同流速下碳纳米管的剪切波色散曲线，图 3(b) 为相应的弯曲波色散曲线. 将图 3 中剪切波色散曲线 (Curve 1) 的最小频率值记为 $\omega_{\min}$，频率区段 $[\omega_{\min}, +\infty]$ 内的状态向量均由两对通带本征向量构成，其物理意义为沿相反传播的两对波.



(a) 碳纳米管能带结构

(a) The energy band structure of SWCNTs without fluid

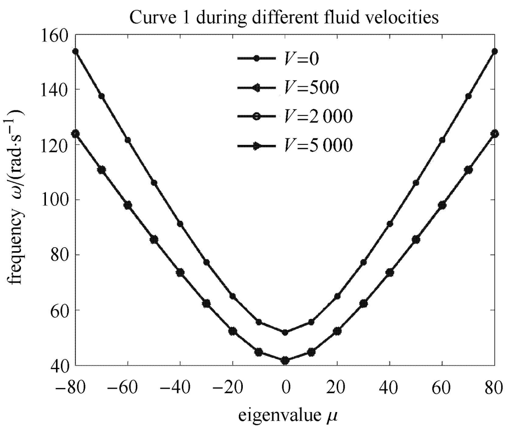


(b) 载流碳纳米管能带结构

(b) The energy band structure of fluid-conveying SWCNTs

图 2 碳纳米管内有无流体频率对比

Fig. 2 Comparison between the energy band structure of SWCNTs with and without fluid

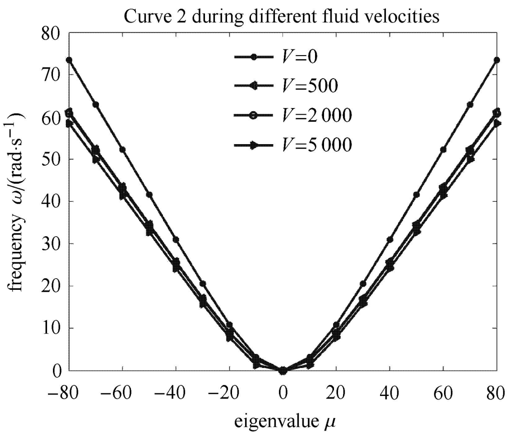


(a) 剪切频率随流体流速变化

(a) Shear frequencies during different fluid velocities

图 3 能带结构随流体流速变化

Fig. 3 The energy band structure during different fluid velocities



(b) 弯曲频率随流体流速变化

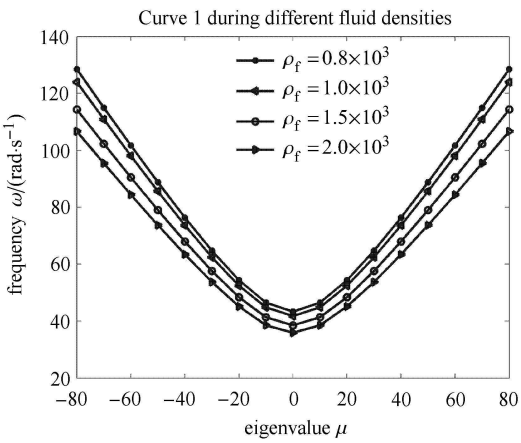
(b) Flexural frequencies during different fluid velocities

图 3 能带结构随流体流速变化 (续)

Fig. 3 The energy band structure during different fluid velocities (continued)

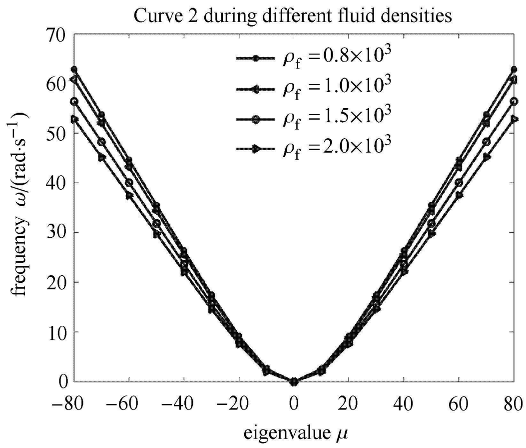
观察图 3 可以发现：随着碳纳米管管内流体流速的增加，载流碳纳米管的弯曲频率与剪切频率均减小. 通过对这一现象的分析，可以得到结论：由于碳纳米管内流体流速的增加，碳纳米管会变得更“柔软”[27]. 这一现象的发生可以由方程 (8) 中的 λ_e 得以解释，因此，在研究载流碳纳米管力学问题时，流速对剪切频率的作用应当考虑.

图 4 描述了碳纳米管能带结构随流体密度变化曲线，其中，图 4(a) 表示不同密度的流体在相同流速 2 000 m/s 下通过碳纳米管时，碳纳米管的剪切波色散曲线；图 4(b) 为弯曲波色散曲线. 将图 4 中剪切波色散曲线 (Curve 1) 的最小频率值记为 $\omega_{\min}$，频率区段 $[0, \omega_{\min}]$ 内的状态向量由一对通带本征向量，



(a) 剪切频率随流体密度变化

(a) Shear frequencies during different fluid density



(b) 弯曲频率随流体密度变化

(b) Flexural frequencies during different fluid density

图 4 能带结构随流体密度变化

Fig. 4 The energy band structure during different fluid density

与一对禁带本征向量构成，通带本征向量表示的物理意义为：一对相反方向传播的波，而禁带本征向量表示的物理意义为：按模态就地振动.

观察图 4 还可以发现：随着碳纳米管管内流体密度的增加，载流碳纳米管的弯曲频率与剪切频率均减小. 通过对这一现象的分析，可以得到结论：由于碳纳米管内流体流速的增加，碳纳米管会变得更“柔软”. 此结论不同于纳伦德拉等 [28] 在非局部弹性理论下的结论. 原因在于本文在哈密顿系统讨论波的传播问题，不同于文献 [28] 的拉格朗日系统. 这一现象的发生可以由方程 (8) 中的 $\lambda_c, \lambda_d, \lambda_e$ 得以解释，因此，在研究载流碳纳米管力学问题时，流体密度对剪切频率的作用应当考虑.

3.2 散射矩阵计算

载流碳纳米管的散射矩阵 [28]

$$\boldsymbol{S}_{ca} = -(\boldsymbol{P}_a - \boldsymbol{K}_r\boldsymbol{Q}_a)^{-1}(\boldsymbol{P}_b - \boldsymbol{K}_r\boldsymbol{Q}_b) \tag{12}$$

表 1 给出了不同频率下的散射矩阵 $\boldsymbol{S}_{ca}$. 研究发现，散射矩阵 $\boldsymbol{S}_{ca}$ 是对称矩酉矩阵，即满足 $\boldsymbol{S}_{ca}^{T} = \boldsymbol{S}_{ca}$ 和 $\boldsymbol{S}_{ca}^{H}\boldsymbol{S}_{ca} = \boldsymbol{I}$. 同时表明：通过载流碳纳米管的入射

表 1 散射矩阵

Table 1 Scattering matrix

ω	$\boldsymbol{S}_{ca}$
100	$\begin{bmatrix} -0.0642+0.9979i & -0.0078-0.0002i \\ -0.0078-0.0002i & 0.0060+1.0000i \end{bmatrix}$
200	$\begin{bmatrix} -0.0345+0.9992i & -0.0190-0.0003i \\ -0.0190-0.0003i & 0.0034+0.9998i \end{bmatrix}$

波功率流等于反射波的功率流，满足功率流守恒的要求，体现了辛方法的优越性.

4 结 论

本文基于辛弹性力学理论和铁木辛柯梁理论，研究了载流碳纳米管的波传播问题. 通过勒让德变换，引入对偶变量，建立了辛体系下的动力学方程；采用波传播分析方法解析得到了载流碳纳米管的能带结构表达式；同时计算了载流碳纳米管的散射矩阵. 此外，可以将本文的方法推广应用到具有周期性结构的二维碳纳米管阵列的能带分析，为纳米机电系统的力学行为研究提供了良好的理论分析方法.

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