T矩阵法在光镊中的应用及进展

王　娟　　任洪亮　　周业鹏

华侨大学信息科学与工程学院, 福建 厦门 361021

摘要　T矩阵法适合用来研究微粒尺寸与入射光波长相近时系统中光镊的捕获力。T矩阵法只取决于散射微粒的形状、尺寸大小、折射率及微粒在坐标系中的位置, 而不受入射场约束。主要简述了T矩阵法基本原理和计算, 综述了光镊中单个微粒、两个微粒及两个以上微粒捕获力和力矩的计算方法, 并对T矩阵法在光镊中的应用前景做了分析。

关键词　光镊; 电磁散射; T矩阵法; 捕获力

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Applications of T-Matrix Method in Optical Tweezers and Its Progress

Wang Juan　　Ren Hongliang　　Zhou Yepeng

College of Information Science & Engineering, Huaqiao University, Xiamen, Fujian 361021, China

Abstract　The trapping force of the optical tweezers is studied using T-matrix method when the particle is in sizes comparable with the wavelength of the incident light. The T-matrix depends only on the composition、size、shape and orientation of particles, independent of the incident field. The basic principles and the calculation methods of T-matrix method are reviewed. The calculations of trapping force and torque of the single particle and two or more particles using T-matrix method are summarized. The prospect provided by T-matrix method for optical tweezers is also analyzed.

Key words　optical tweezers; electromagnetic scattering; T-matrix method; trapping force

OCIS codes　350.4855; 290.5850; 200.4860; 290.5825; 260.2160

1　引　　言

　　光镊依靠光的梯度力形成, 被形象地描绘成"光捕获阱"或"光学势阱"等物理术语, 由于其能够无损伤、非机械接触地捕获和操纵微粒, 自1986年诞生以来, 就被广泛地应用于金属粒子[1]、生物活细胞和细胞器的微操控研究[2-7]。当微粒尺寸与入射光波长相近时, 通常将光镊中光与微粒的相互作用看作电磁散射, 并可通过麦克斯韦方程来求解散射场。计算电磁散射场的方法有: 广义洛伦兹-米理论(GLMT)[8-9], 有限元法(FEM)[10-11], 时域有限差分法(FDTD)[12-14], 离散偶极子近似法(DDA)[15]和T矩阵法(T-matrix method)[16]等, 这些数值计算方法有各自的优缺点, 计算时所要满足的边界条件各不相同。T矩阵法是简单而有效的计算方法[17], 具有一定的优越性。Mishchenko等[18]就Waterman对T矩阵的贡献做了简短介绍。Mishchenko等[17,19-22]汇总了2004年至2013年间各领域发表的有关T矩阵的论文, 并整合成一个综合性数据库, 该数据库现已更新到第五期, 是不同领域学者很好的参考资料。本文对T矩阵法的基本原理和计算, T矩阵法用于计算光镊中单个球形、非球形微粒、两个球形微粒的捕获力及力矩等情况进行了综述。

2　散射场的数值计算方法

　　光散射场的数值计算方法主要有FEM、FDTD、DDA、GLMT和T矩阵法, 它们的计算步骤及优缺点如表1所示。

表 1 电磁散射场的几种数值计算方法的比较

Table 1 Comparison of numerical computation methods of electromagnetic scattering field

Method	Calculation steps	Advantage	Disadvantage
FEM	1、 The optical tweezers is considered as the electromagnetic field source changing with time. 2、The 3−D computation domain is discretized into a fine mesh of points. A stability criterion is set an upper boundary between the grid spacing of the mesh and the time step. 3、 Iterations the field of the particles. 4、The force is calculated.	1、The theory is simple and can be used to calculate arbitrary shape and random component particles. 2、 The calculation is accuracy.	1、 The amount of calculation is increased rapidly when the particle volume is increased, so it often can be used to calculate the small particles. 2、 The amount of calculation is increased rapidly when the integral space is more accurately. 3、 The far− field effect and boundary conditions cannot be ignored. 4、The entire process can be recalculated when the particle which composition and orientation is changed in the optical tweezers.
FDTD	1、The space is discretized into a fine mesh. 2、Iterations the field between the grid spacing of the mesh and the time step. 3、According to the distribution of electromagnetic field, the radial force is calculated using Lorentz force and electromagnetic tensor.		
DDA	1、 The particles trapped in the optical tweezers are discretized into a cubic array of polarizable points with each point representing a dipole. 2、 The scattering field of each dipole is calculated. 3、 The moment and the force of each dipole are calculated, and it can be obtained the total force of the particle when iterating all of the dipoles in the optical tweezers.	1、 The method needs not be considered the boundary condition of electromagnetic fields. 2、It can be used to deal with any arbitrary shape and refractive index distribution of the particles. 3、It is can be used to two or more trapped particles in the optical tweezers. 4、 There are lots of software and program codes describe to DDA.	1、 The amount of calculation of the method is relatively large. 2、The entire process is recalculated when the particle which composition and orientation is changed in the optical tweezers.

表 1 电磁散射场的几种数值计算方法的比较

续表1

Method	Calculation steps	Advantage	Disadvantage
GLMT	1、The corresponding boundary conditions of scattering problems must be solved. 2、The Mie coefficients and the beam-shape coefficients are calculated. 3、The scattering cross section of different particles is calculated. 4、The radiation trapping force is calculated.	The exact solutions can be obtained from the Maxwell´s equations.	Many Mie coefficients and beam-shape coefficients are required for the computation of the trapping force becomes laborious, when the size of the trapped particle is comparable to or larger than the laser wavelength.
T-matrix method	1、The T-matrix elements of the particles are calculated. 2、The incident and scattering fields can be expanded in terms of regular vector spherical wave functions. 3、The incident expansion coefficients are calculated. 4、The scattering expansion coefficients are calculated using the T matrix and incident expansion coefficients. 5、The force and torque are calculated.	1、The T-matrix depends only on the particle composition, size, shape, orientation and the wavelength of the incident field. 2、For any particular particles, the T-matrix only needs to be calculated once. 3、It is attractive method for describing optical micromanipulation.	The theory of the T-matrix method is simple.

3　T矩阵法

3.1　T矩阵法基本原理

光镊中,在所要计算的位置及方向上,将入射光束分解为球面矢量波:

$$E_{\mathrm{inc}} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [a_{nm} f_{nm}^{\mathrm{RgM}}(k\boldsymbol{r}) + b_{nm} f_{nm}^{\mathrm{RgN}}(k\boldsymbol{r})] , \tag{1}$$

式中球面矢量波函数 f_{nm}^{RgM} , f_{nm}^{RgN} 可分别表示为:

$$f_{nm}^{\mathrm{RgM}}(k\boldsymbol{r}) = (-1)^{m} d_{n} \exp(im\phi) \mathrm{j}_{n}(kr) C_{nm}(\theta) , \tag{2}$$

$$f_{nm}^{\mathrm{RgN}}(k\boldsymbol{r}) = (-1)^{m} d_{n} \exp(im\phi) \times \left\{ \frac{n(n+1)}{k\boldsymbol{r}} \mathrm{j}_{n}(kr) P_{nm}(\theta) + \left[\mathrm{j}_{n-1}(kr) - \frac{n}{kr} \mathrm{j}_{n}(kr) \right] B_{nm}(\theta) \right\} , \tag{3}$$

式中 $\mathrm{j}_{n}(kr)$ 是球谐贝塞尔函数, d_{n} 是归一化常数, $B_{nm}(\theta)$, $C_{nm}(\theta)$, $P_{nm}(\theta)$ 均是角相关矢量球谐函数,其表达式分别为:

$$\begin{cases} B_{nm}(\theta) = \hat{\theta} \dfrac{\mathrm{d}}{\mathrm{d}\theta} d_{0m}^{n}(\theta) + \hat{\phi} \dfrac{im}{\sin\theta} d_{0m}^{n}(\theta), \\ C_{nm}(\theta) = \hat{\theta} \dfrac{\mathrm{d}}{\mathrm{d}\theta} d_{0m}^{n}(\theta) - \hat{\phi} \dfrac{im}{\sin\theta} d_{0m}^{n}(\theta), \\ P_{nm}(\theta) = \hat{\theta} d_{0m}^{n}(\theta), \\ d_{n} = \left[\dfrac{2n+1}{4\pi n(n+1)} \right]^{1/2}, \end{cases} \tag{4}$$

式中 $d_{0m}^{n}(\theta)$ 是魏格纳 d 函数。

散射场同样可用球面矢量波来表示,其表达式为:

$$E_{\text{scat}} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [p_{nm} M_{nm}(k\boldsymbol{r}) + q_{nm} N_{nm}(k\boldsymbol{r})] \ , \tag{5}$$

式中 $M_{nm}(k\boldsymbol{r}), N_{nm}(k\boldsymbol{r})$ 是用第一类球汉克尔函数 $\mathrm{h}_n^{(1)}(k\boldsymbol{r})$ 分别代替 $f_{nm}^{\mathrm{RgM}}(k\boldsymbol{r})$，$f_{nm}^{\mathrm{RgN}}(k\boldsymbol{r})$ 中的球贝塞尔函数得到。麦克斯韦方程具有线性性质，因此入射场和散射场的展开系数之间存在一定的线性关系，现将 a_{nm}, b_{nm} 简写为 $\boldsymbol{a}$ 和 $\boldsymbol{b}$；p_{nm}, q_{nm} 简写为 $\boldsymbol{p}$ 和 $\boldsymbol{q}$，其线性关系可用 T 矩阵来表示：

$$\begin{bmatrix} \boldsymbol{p} \\ \boldsymbol{q} \end{bmatrix} = \boldsymbol{T} \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{bmatrix} = \begin{bmatrix} \boldsymbol{T}^{11} & \boldsymbol{T}^{12} \\ \boldsymbol{T}^{21} & \boldsymbol{T}^{22} \end{bmatrix} \begin{bmatrix} \boldsymbol{\alpha} \\ \boldsymbol{\beta} \end{bmatrix} \ , \tag{6}$$

$$p_{nm} = \sum_{n'm'} (T_{nmn'm'}^{11} a_{n'm'} + T_{nmn'm'}^{12} b_{n'm'}) \ , \tag{7}$$

$$q_{nm} = \sum_{n'm'} (T_{nmn'm'}^{21} a_{n'm'} + T_{nmn'm'}^{22} b_{n'm'}) \ . \tag{8}$$

3.2　T矩阵的计算

Fikioros 和 Waterman[23]是 GLMT 的先驱，1960 年 Waterman[24]报道了计算 T 矩阵的步骤，并于 1965 年首次[25]提出了 T 矩阵法。计算 T 矩阵的方法主要有 FDTD[26]、DDA[27]、点匹配法(PMM)[28]和扩展边界条件法

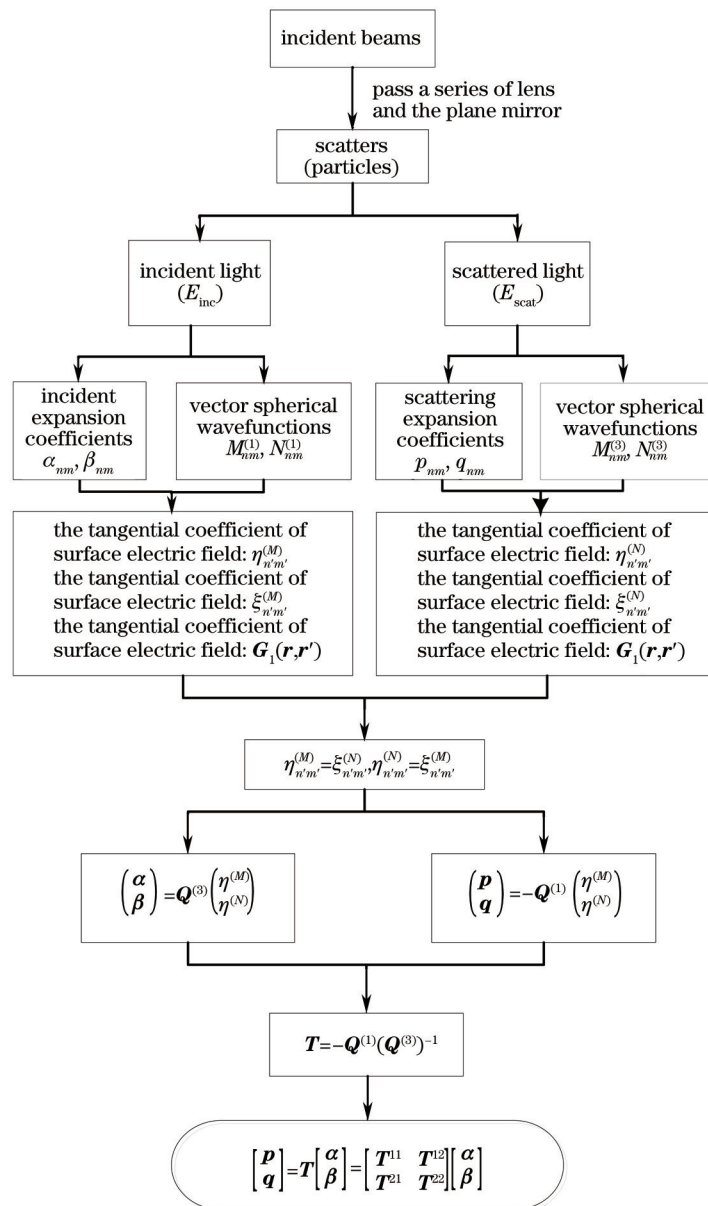图 1　EBCM 计算 T 矩阵的流程图

Fig.1　Flow diagram of T-matrix calculation using EBCM

(EBCM)[29]。EBCM 又叫零场法(NFM)或矩阵法(TMM)[30],是计算 T 矩阵最常用的一种方法,图 1 以高斯光束为入射光束介绍了计算 T 矩阵的流程图。EBCM 仅适用于均匀且各向同性的对称球形微粒,微粒尺寸较大时其运算速度会很慢。微粒不对称时,Loke 等[31]于 2009 年提出用 PMM 计算 T 矩阵,这种方法避免了 EBCM 对整个微粒进行时间积分,弥补了 EBCM 的不足。

4　T矩阵法的应用

4.1　T矩阵法用于单体计算

光镊中,T 矩阵法用于单体研究的论文居多,其理论计算也较为成熟。Nieminen 等[32]利用 MATLAB 软件构建了计算光镊的工具箱,提出光散射问题可用 T 矩阵法精确计算。后来利用 T 矩阵法,对单个微粒和复合微粒的捕获力及力矩进行了计算,将其在光镊模型中的应用做了总结[33]。Mishchenko 等[34-35]对微粒电磁散射的 T 矩阵法及其应用等进行了总结,并建立了数据库。光镊中微粒捕获力是矢量,其计算可表示为:

$$F = \frac{nPQ}{c} , \tag{9}$$

式中 P 为入射光功率,若使计算更精确,可用 $P = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \left(|a_{nm}|^2 + |b_{nm}|^2 \right)$ 来计算,c 为自由空间光速,Q 为捕获效率(捕获因子),轴向捕获效率 Q_z 为:

$$Q_z = \frac{2}{P} \sum_{n=1}^{\infty} \sum_{m=-n}^{n} \frac{m}{n(n+1)} \mathrm{Re}\left(a_{nm}^* b_{nm} - p_{nm}^* q_{nm} \right) - \frac{1}{n+1} \cdot \left[\frac{n(n+1)(n-m+1)(n+m+1)}{(2n+1)(2n+3)} \right]^{1/2} \times \tag{10}$$
$$\mathrm{Re}\left(a_{nm} a_{n+1,m}^* + b_{nm} b_{nm}^* - p_{nm} p_{nm}^* - q_{nm} q_{nm}^* \right)$$

光镊中力矩可表示为:

$$\Gamma = \frac{p}{\omega} \tau , \tag{11}$$

式中 ω 为入射光频率,力矩效率 τ 为:

$$\tau = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} m \left(|a_{nm}|^2 + |b_{nm}|^2 - |p_{nm}|^2 - |q_{nm}|^2 \right) / P . \tag{12}$$

4.1.1　均匀球形微粒

均匀球形微粒结构简单,如手柄等,其捕获力计算方便,光镊中单个均匀球形微粒的 T 矩阵是对角矩阵,该结果由 Waterman[36]给出,并将其数值结果与实验结果进行了对比,球坐标系中 T 矩阵可写为:

$$T = \begin{bmatrix} T^{(11)} & 0 \\ 0 & T^{(22)} \end{bmatrix} , \tag{13}$$

其对角元素为:

$$T_{nmn'm'}^{(11)} = \delta_{nn'} \delta_{mm'} T_n^{(M)} = -\frac{\mathrm{j}_n(k_s a)[ka\mathrm{j}_n(ka)]' - \mathrm{j}_n(ka)[k_s a\mathrm{j}_n(k_s a)]'}{\mathrm{j}_n(k_s a)[ka\mathrm{h}_n(ka)]' - \mathrm{h}_n(ka)[k_s a\mathrm{j}_n(k_s a)]'} , \tag{14}$$

$$T_{nmn'm'}^{(22)} = \delta_{nn'} \delta_{mm'} T_n^{(N)} = -\frac{\frac{k_s^2}{k^2} \mathrm{j}_n(k_s a)[ka\mathrm{j}_n(ka)]' - \mathrm{j}_n(ka)[k_s a\mathrm{j}_n(k_s a)]'}{\frac{k_s^2}{k^2} \mathrm{j}_n(k_s a)[ka\mathrm{h}_n(ka)]' - \mathrm{h}_n(ka)[k_s a\mathrm{j}_n(k_s a)]'} . \tag{15}$$

Nieminen 等[28]系统地对强聚焦激光束进行了研究,Bareil 等[37]对数值孔径为 1.20 的高阶修正强聚焦矢量高斯光束光镊进行了模拟实验。若均匀球形微粒为旋转对称球形微粒,T 矩阵是 n 阶对角阵,文献[38]中有计算 n 阶对角 T 矩阵的具体公式,用计算机编程可实现对这种 T 矩阵的计算,这为复杂粒子的研究奠定了扎实的基础。

4.1.2　非球形微粒

非球形微粒本身形状各异,研究光镊捕获该种微粒的过程比较复杂,如酵母细胞等生物微粒,而这刚好是吸引研究者进行探索的原因。不同作者利用 T 矩阵法对随机球状体微粒[39]、旋转椭球体[40]、纳米圆柱体[41]、超椭球和圆角立方体[42]等非球形微粒进行了理论计算与模拟。对非球形微粒的计算,除入射场和散射场外

还要进行内场的计算[43]，其内场可表示为：

$$E_{\text{int}} = \sum_{n=1}^{\infty} \sum_{m=-n}^{n} [c_{nm} f_{nm}^{\text{RgM}}(m_r k r) + d_{nm} f_{nm}^{\text{RgN}}(m_r k r)],$$ (16)

式中 m_r 是微粒内部折射率，c_{nm}、d_{nm} 是内场展开系数。

　　光镊对非球形微粒的捕获如图2所示。T矩阵法是一种求解电磁散射捕获力的有效方法[43]，利用T矩阵法可计算圆柱体和类球体微粒在平面波光镊中的辐射力，及电磁散射场中任意形状和结构微粒的力及力矩[44]；计算旋转对称但横轴与纵轴比率不同的非球形微粒的光散射过程；还可用于研究(如图3所示)非轴对称、不同参数的超椭球体微粒[42]，并得出不同球体散射截面随散射角变化的值(如图4所示)。Nieminen 等[45]编写了一套可用于GLMT和T矩阵计算辐射力的程序。Mishchenko 等[46-47]对T矩阵法的程序代码细节问题做了小结。徐飞等[48]利用超椭球方程描述粒子形状，用MATLAB实现了粒子形状的绘制和表面离散化，通过T矩阵法计算了非球形粒子的散射特性，并将其结果与Mie散射结论进行对比，得出T矩阵法计算非球形微粒的可靠性。Xu 等[49]利用T矩阵法计算了旋转椭球微粒微观物理参数的光散射特性，其计算结果与FDTD的相同。

图2 光镊捕获非球形微粒

Fig.2 Non-spherical particle trapped in optical tweezers
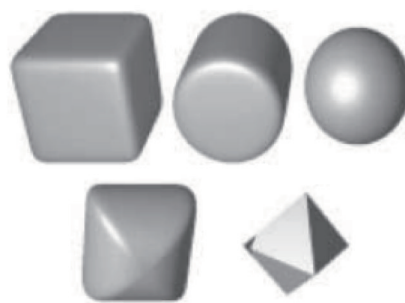

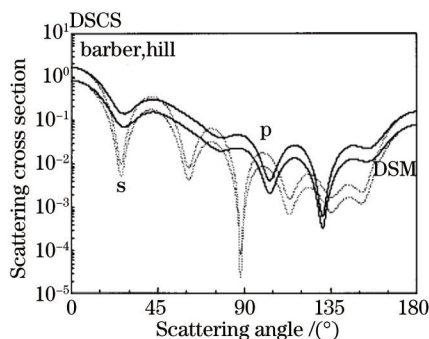图3 不同参数的超椭球体

Fig.3 Superellipsoids with different parameters

图4 不同非球形微粒截面随散射角变化的值

Fig.4 Scattering cross section of different non-spherical particles versus scattering angle

　　除了利用T矩阵法研究了任意形状和结构的微粒外，张良福课题组[50]还对非球形气溶胶微粒的短波红外特性进行了研究。Forestiere课题组[30]提出将T矩阵算法与现代图形处理单元(GPUs)相结合，并模拟了纳米光学材料和任意形状粒子凝聚体的光散射问题。Yang课题组[39]用不变量嵌入法(IIM)有效实现了T矩阵的计算，并与标准分离变量法(SOV)结合对较大的非均匀球形微粒进行了模拟计算。

4.1.3 多层球微粒

　　对多层球微粒的研究是大多数学者感兴趣之处，如生物细胞包括细胞壁、细胞膜和细胞核等多层结构，要将其研究得比较清楚，理论计算与数值模拟都会非常复杂。T矩阵法可计算双层球多次散射及多层球的电磁散射问题，Peterson 等[51]证明了T矩阵法还可用于计算更多形状多层散射体电磁散射问题。Cao 等[52]提出一种新的T矩阵法来计算多层球的散射问题(如图5所示)，每层球面可用标量磁导率和介电常数来表示，球内外的电磁场展开成一系列球谐函数，并与傅里叶变换形式的结果进行对比。图6是电场平面与磁场平面上，5层等离子体球壳的雷达散射截面(RCS)值随散射角的变化。

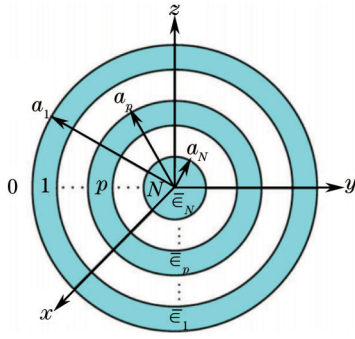　　对多层球而言，每层的折射率不同，光束照射微粒后每层的散射场与内场就有很大差别，多层球T矩阵

图 5　多层球微粒模型

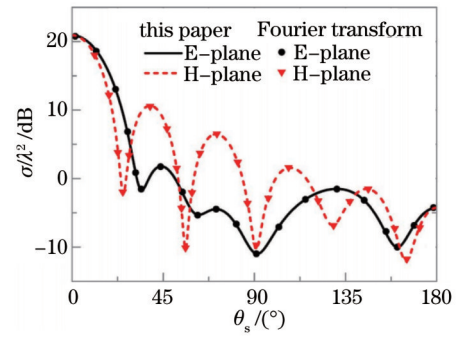Fig.5　Multilayer particles modeling

图 6　电场与磁场平面上 5 层等离子体球 RCS 值随散射角的变化曲线

Fig.6　RCS values of a 5-layer plasma spherical shell versus scattering angle in E- and H-planes

的计算也是通过比较入射场、散射场与内场的展开系数间的关系求得。对于内层折射率为 m_1，外层折射率为 m_2 的双层球微粒[47,51,53-54]，其 T 矩阵的计算为：

$$T = -B \times A^{-1} = -\left[B_2 \times BB_2 \times \left(-B_1 \times A_1^{-1}\right)\right] \times \left[A_2 + AA_2 \times \left(-B_1 \times A_1^{-1}\right)\right]^{-1},\tag{17}$$

式中对矩阵元 B_2，BB_2，A_2，AA_2 及 $(-B_1 \times A_1^{-1})$ 的计算也有详细描述[53-54]。

求得 T 矩阵后，随机取向的非球形微粒的散射特性可通过解析式直接求得，这种计算方法比对所有取向求平均值的方法快几十倍[47]。其中消光截面和散射截面分别表示为：

$$C_{ext} = -\frac{2\pi}{k^2} \mathrm{Re} \sum_{n-1}^{\infty} \sum_{m=-n}^{n} \left[T_{nmnm}^{11} + T_{nmnm}^{12}\right],\tag{18}$$

$$C_{scat} = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} \sum_{n'=1}^{\infty} \sum_{m=-n}^{n} \sum_{m'=-n'}^{n'} \sum_{i=1}^{2} \sum_{j=1}^{2} \left|T_{nmn'm'}^{ij}\right|^2.\tag{19}$$

入射光和散射光可由 Stokes 矢量 I_s 和 I_i 来描述，其关系式可由 Müller 矩阵来表述，其表达式为：

$$I_s = \frac{C_{scat}}{4\pi R^2} F(\theta) I_i,\tag{20}$$

式中 R 为散射体到观察点的距离。Müller 矩阵是描述散射体对入射光的散射影响，对于轴对称的非球形微粒，Müller 矩阵只有 6 个独立的元素[47]：

$$F(\theta) = \begin{bmatrix} F_{11}(\theta) & F_{12}(\theta) & 0 & 0 \\ F_{12}(\theta) & F_{22}(\theta) & 0 & 0 \\ 0 & 0 & F_{33}(\theta) & F_{34}(\theta) \\ 0 & 0 & -F_{34}(\theta) & F_{44}(\theta) \end{bmatrix},\tag{21}$$

式中 F_{11} 是单次散射相函数，满足归一化条件：

$$\frac{1}{2} \int_0^\pi F_{11}(\theta) \sin\theta \mathrm{d}\theta = 1,\tag{22}$$

不对称因子 g 反映了微粒散射各向异性的程度，其表达式为：

$$g = \langle \cos\theta \rangle = \frac{1}{2} \int_{-1}^{1} \cos\theta F_{11}(\theta) \mathrm{d}\cos\theta,\tag{23}$$

当 $g=0$ 时为各向同性微粒。

同样，多层球有不同的形状，特别是生物细胞或者含有核的微粒，可按如图 7 所示的模型进行分析研究[55]。孙贤明等[53]基于 T 矩阵法，以含核椭球粒子为模型，计算了其内核(黑炭)的散射特性，分析了核的大小和形状对消光系数、散射系数、吸收系数及 Müller 矩阵等参数的影响，模拟并分析了散射角对 Müller 矩阵等的影响。

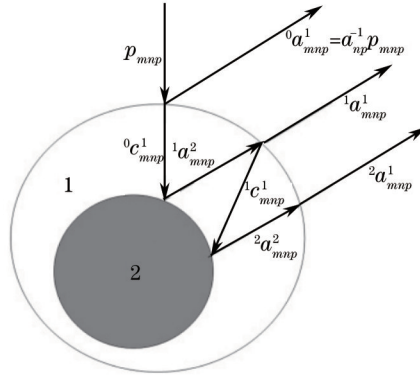综上所述，T 矩阵法对单个球形微粒捕获力的计算是非球形微粒与多层球微粒的基础，因而作为椭球体的酵母细胞、饼状的动物红细胞及类球体的动植物细胞等均可被实验研究，这样就能很好地将理论与实验结合，为光镊在生物学中的应用进一步拓展空间。

图 7　含核微粒模型

Fig.7　Model of core-shell particle

4.2　T矩阵用于多微粒计算

光镊可以用来捕获两个及多个微粒,该种情况下捕获力的计算没有精确解。Peterson 等[56]首先给出了用 T 矩阵法求多个微粒的散射解,图 8 是存在两个微粒的 T 矩阵光散射示意图[56],可以看出入射光束方向不同时,散射光束存在多种可能情况,该图为光镊中多微粒的研究提供很好的思路。

2005 年,Xu 等[57]用几何光学方法研究了光镊中两个微粒的轴向捕获力,其思路是让入射光先通过一个微粒后再通过第二个微粒,该种方法仅适用于入射光波长远小于微粒尺寸的情况。同年,白璐等[58]采用 GLMT 对高斯入射波束下串粒子的散射问题做了研究。若系统入射波 E_{inc} 为平面波,用 T 矩阵法计算如图 9 所示。
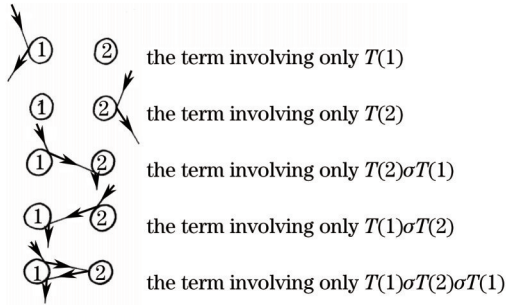

图 8　两个微粒的光散射示意图

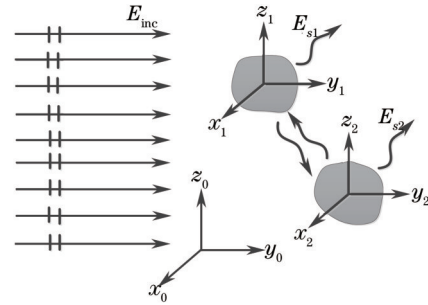Fig.8　Model of scattering light with two particles

图 9　平面波入射下两微粒的电场分布图

Fig.9　Electric field distributions of two particles illuminated by plane wave

系统坐标系定为坐标 0,微粒 1 和微粒 2 的坐标系分别定为坐标 1 和坐标 2,设微粒 1 和微粒 2 的散射波在各自坐标系下分别为 E_{s1} 和 E_{s2},则空间总场写成波函数的形式为:

$$E_t(r_0,r) = \psi^{(1)}(r_0,r)\cdot a + \psi^{(3)}(r_1,r)\cdot b_1 + \psi^{(3)}(r_2,r)\cdot b_2 , \qquad (24)$$

式中 b_1 和 b_2 分别是散射体 1 和散射体 2 的散射波分量,利用矢量波函数加法定理和 T 矩阵的定义求得:

$$b_1 = \left[I - T_{1(I)}\cdot A_{1,2}\cdot T_{2(I)}\cdot A_{2,1} \right]^{-1}\cdot T_{1(I)}\cdot\left[B_{1,0} + A_{1,2}\cdot T_{2(I)}\cdot B_{2,0} \right]\cdot a , \qquad (25)$$

$$b_2 = \left[I - T_{2(I)}\cdot A_{2,1}\cdot T_{1(I)}\cdot A_{1,2} \right]^{-1}\cdot T_{2(I)}\cdot\left[B_{2,0} + A_{2,1}\cdot T_{1(I)}\cdot B_{1,0} \right]\cdot a , \qquad (26)$$

(25)~(26)式中 $T_{i(n)}$ 形式表示 n 个散射体时,第 i 个散射体的 T 矩阵。当 $n=1$ 时,即为单体散射的 T 矩阵。由 (25)式和(26)式可以定义新的 T 矩阵为:

$$b_1 = T_{1(2)}\cdot B_{1,0}\cdot a , \qquad (27)$$

$$b_2 = T_{2(2)}\cdot B_{2,0}\cdot a , \qquad (28)$$

$$T_{1(2)}\cdot B_{1,0} = \left[I - T_{1(I)}\cdot A_{1,2}\cdot T_{2(I)}\cdot A_{2,1} \right]^{-1}\cdot T_{1(I)}\cdot\left[B_{1,0} + A_{1,2}\cdot T_{2(I)}\cdot B_{2,0} \right] , \qquad (29)$$

$$T_{2(2)}\cdot B_{2,0} = \left[I - T_{2(I)}\cdot A_{2,1}\cdot T_{1(I)}\cdot A_{1,2} \right]^{-1}\cdot T_{2(I)}\cdot\left[B_{2,0} + A_{2,1}\cdot T_{1(I)}\cdot B_{1,0} \right] , \qquad (30)$$

式中 $T_{i(2)}$ 是第 i 个散射体在有两个散射体时的T矩阵,它将第 i 个散射体在有两个散射体存在时的总散射场与入射场联系起来。使新的T矩阵仍然是相对于散射体本身的坐标而定义的转移因子 $B_{i,0}$。这两种思路和方法可直接用于聚焦光束形成的光镊中,对今后在光镊中求两个及多个微粒的散射解奠定了基础。

Mishchenko 等[59]用 T 矩阵法得到了多分散系中离散自由介质相干反向散射的精确结果,同年,Mackowski 等[60]也利用 T 矩阵对多球系统的散射和吸收特性进行了研究(如图10所示)。Cui[61]利用 T 矩阵法计算了冷原子气体中两体及三体的散射问题。
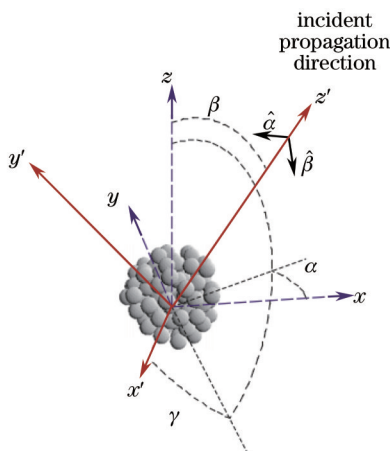

图10 多分散系的电磁散射

Fig.10 Electromagnetic scattering of discrete random medium

可以看出光镊系统中多微粒的研究仍然是一个热点,但对其使用 T 矩阵法计算捕获力的理论还不够成熟,至今没有精确的数值解,这将是继续研究光镊捕获微粒的一个方向,因为多细胞融合与分解是研究生物细胞技术的基础,而多分散系在化学研究中占很重要的地位。

4.3 T矩阵法用于其他类型光镊

目前产生了全息光镊、光纤光镊等许多衍生光镊技术,这些衍生光镊在多微粒操纵方面具有很大优势。全息光镊[62-63]形成的光场性质不同,可实现不同的功能,如单粒子旋转、多粒子操控和分选等。Grier[64]预言了全息光镊技术将引发光学操纵的技术革命。Simpson 等[65]用 T 矩阵法计算了全息光镊微粒间的相互作用力,并分析了高斯光束中类球体的辐射力[66]。Horst 等[67]证明动态全息光镊可研究纳米结构的细胞和弹性蛋白网络等。

光纤光镊的捕获光路和观测光路分离,操纵灵活,结构简单,捕获范围大。Liu 等[68]研究了锥形光纤光镊的构建和应用,并计算了微粒的受力。Gong 等[69]对渐变折射率多模光纤光镊进行了数值模拟和实验捕获。光纤光镊还可用于生物细胞的捕获和输送[70]。多微粒操纵可用这些衍生光镊技术来实现,若与理论计算相结合,光镊技术的精确性与实际应用的广泛性均可进一步得到提升。

5　结　论

T矩阵法是一种通用、精确、有效的理论方法,已被广泛应用于光镊中单个微粒、两个微粒及随机离散介质表面微粒的电磁散射性质、捕获力及力矩的计算。尤其是在微粒尺寸与入射光波长相近的情况下,常采用T矩阵法计算。计算T矩阵的常用方法有 FDTD、DDA、EBCM、IIM 和 PPM。本文针对 T 矩阵法的原理和计算、T 矩阵法计算光镊中不同形状、大小微粒的力和力矩做了小结。随着 T 矩阵法在光镊中的应用日渐成熟,并且光镊结构趋于多样化,今后 T 矩阵法将用于光镊捕获多微粒、光纤光镊及全息光镊的数值计算中,为光镊在分子生物学、胶体化学和实验原子物理等领域的应用提供理论指导。

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