

General Expression Analysis of the Hamiltonian Operator and Its Formula

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Abstract

The Hamiltonian operator ∇ and the common expressions such as the Laplacian operator, gradient, divergence, and curl generated by it are not the same in different curve coordinate systems. This paper defines a three-dimensional orthogonal curve coordinate system (u_1, u_2, u_3) , introducing coordinate factor h_1, h_2, h_3 , deriving the general form of $\nabla, \nabla\phi, \nabla \cdot A, \nabla \times A, \nabla^2$, and the general expression of Poisson equation as well as Laplace equation.

Keywords

Hamiltonian Operators, Laplacian Operator, Gradient, Divergence, Curl

哈密顿算符及其一般运算表达式的分析

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摘要

哈密顿算符 ∇ 及其产生的拉普拉斯算符、梯度、散度和旋度常见运算式在不同曲线坐标系中具体表达式不相同。本文通过定义一个三维正交曲线坐标系 (u_1, u_2, u_3) , 引入坐标因子 h_1, h_2, h_3 , 推导得到了关于 $\nabla, \nabla\phi, \nabla \cdot A, \nabla \times A, \nabla^2$ 的一般形式及Poisson方程和Laplace方程的一般表达式。

关键词

哈密顿算符, 拉普拉斯算符, 梯度, 散度, 旋度

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1. 引言

哈密顿算符 ∇ 是关于空间的一阶偏微分算子, 在数学和物理学中发挥着重要作用。由 ∇ 可以产生一系列的偏微分方程, 如泊松方程、拉普拉斯方程等, 这些方程在电磁学、热传导等方面经常用到[1] [2] [3]。 ∇ 及其产生的梯度、散度和旋度等常见运算式在笛卡尔坐标系、柱坐标系、球坐标系、和极坐标系下, 其具体表达形式是不一样的, 能不能给各种运算式找到一个通用的一般表达式来统一呢? 本文针对这个问题做了一些分析, 在三维正交曲线坐标系 (u_1, u_2, u_3) 下, 得到了几个包含哈密顿算符运算式的一般表达式。

2. 正交曲线坐标系

考虑一个由三维正交曲线坐标系 (u_1, u_2, u_3) [4]组成的空间, 其中一个无限小的体积元可由 $u_1, u_1 + du_1, u_2, u_2 + du_2, u_3, u_3 + du_3$ 相围得到。一般通过 u_1, u_2, u_3 乘以坐标因子 h_1, h_2, h_3 来表示三个方向的距离, h_1, h_2, h_3 是 (u_1, u_2, u_3) 的函数。

如图 1 所示, 定义三个线元:

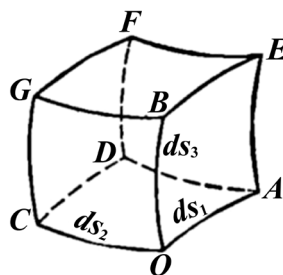


Figure 1. The map of generalized coordinates volume element

图 1. 广义坐标系体积元图

$$ds_1 = h_1 du_1, \quad ds_2 = h_2 du_2, \quad ds_3 = h_3 du_3 \quad (1.1)$$

体积元 $dV = ds_1 ds_2 ds_3 = h_1 h_2 h_3 du_1 du_2 du_3$, 则哈密顿算符可以表示为:

$$\nabla = \frac{\partial}{\partial s_1} \mathbf{e}_1 + \frac{\partial}{\partial s_2} \mathbf{e}_2 + \frac{\partial}{\partial s_3} \mathbf{e}_3 = \frac{\partial}{h_1 \partial u_1} \mathbf{e}_1 + \frac{\partial}{h_2 \partial u_2} \mathbf{e}_2 + \frac{\partial}{h_3 \partial u_3} \mathbf{e}_3 \quad (1.2)$$

$\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ 分别是空间变量 (u_1, u_2, u_3) 的单位矢量。

1) 一标量 ϕ 在正交曲线坐标系 (u_1, u_2, u_3) 连续, 一阶微分存在, 则根据梯度的定义式, ϕ 的梯度分量:

$$\frac{\partial \phi}{\partial s_1} = \frac{\partial \phi}{h_1 \partial u_1}, \quad \frac{\partial \phi}{\partial s_2} = \frac{\partial \phi}{h_2 \partial u_2}, \quad \frac{\partial \phi}{\partial s_3} = \frac{\partial \phi}{h_3 \partial u_3} \quad (1.3)$$

$$\nabla\phi = \left(\frac{\partial\phi}{h_1\partial u_1}\right)\mathbf{e}_1 + \left(\frac{\partial\phi}{h_2\partial u_2}\right)\mathbf{e}_2 + \left(\frac{\partial\phi}{h_3\partial u_3}\right)\mathbf{e}_3 \quad (1.4)$$

2) 一矢量 A 在正交曲线坐标系 (u_1, u_2, u_3) 连续, 一阶微分存在, 那么矢量 A 穿过面 OCGB 和 ADFE 的向外通量为:

$$\frac{\partial}{\partial s_1}(A_1 ds_2 ds_3) ds_1 = \frac{\partial}{\partial u_1}(h_2 h_3 A_1) du_1 du_2 du_3 = \frac{1}{h_1 h_2 h_3} \frac{\partial}{\partial u_1}(h_2 h_3 A_1) dV \quad (1.5)$$

用同样的方法可以得到穿过其他 4 个平面的通量, 则根据散度的定义, A 的散度:

$$\operatorname{div}A = \nabla \cdot A = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial u_1}(h_2 h_3 A_1) + \frac{\partial}{\partial u_2}(h_3 h_1 A_2) + \frac{\partial}{\partial u_3}(h_1 h_2 A_3) \right] \quad (1.6)$$

3) 矢量 A 是 (u_1, u_2, u_3) 的函数, 在正交曲线坐标下连续可微, A_1 、 A_2 、 A_3 是沿着 u_1 、 u_2 、 u_3 三个变量方向上的分量, 由 Stokes 定理, 在面 OADC 上 A_1 沿着边 OA 和 DC 的线积分等于:

$$\left[h_1(u_1, u_2) A_1(u_1, u_2) - h_1(u_1, u_2 + du_2) A_1(u_1, u_2 + du_2) \right] du_1 = -\frac{\partial(h_1 A_1)}{\partial u_2} du_1 du_2 \quad (1.7)$$

沿着边 AD 和 CO 的线积分等于

$$\left[h_2(u_1 + du_1, u_2) A_2(u_1 + du_1, u_2) - h_2(u_1, u_2) A_2(u_1, u_2) \right] du_2 = \frac{\partial(h_2 A_2)}{\partial u_1} du_1 du_2 \quad (1.8)$$

根据 Stokes 定理, A 沿着面 OADC 边界上的环路积分等于 $\nabla \times A$ 穿过平面 OADC 的通量, 即:

$$(\nabla \times A)_3 = \frac{1}{h_1 h_2} \left[\frac{\partial(h_2 A_2)}{\partial u_1} - \frac{\partial(h_1 A_1)}{\partial u_2} \right] \quad (1.9)$$

对于另外两个面 OBGC 和 OAEB 也可以得到

$$(\nabla \times A)_1 = \frac{1}{h_2 h_3} \left[\frac{\partial(h_3 A_3)}{\partial u_2} - \frac{\partial(h_2 A_2)}{\partial u_3} \right] \quad (1.10)$$

$$(\nabla \times A)_2 = \frac{1}{h_3 h_1} \left[\frac{\partial(h_1 A_1)}{\partial u_3} - \frac{\partial(h_3 A_3)}{\partial u_1} \right] \quad (1.11)$$

所以, 矢量 A 的旋度为

$$\begin{aligned} \operatorname{curl}A &= \nabla \times A \\ &= \frac{1}{h_2 h_3} \left[\frac{\partial(h_3 A_3)}{\partial u_2} - \frac{\partial(h_2 A_2)}{\partial u_3} \right] \mathbf{e}_1 + \frac{1}{h_3 h_1} \left[\frac{\partial(h_1 A_1)}{\partial u_3} - \frac{\partial(h_3 A_3)}{\partial u_1} \right] \mathbf{e}_2 \\ &\quad + \frac{1}{h_1 h_2} \left[\frac{\partial(h_2 A_2)}{\partial u_1} - \frac{\partial(h_1 A_1)}{\partial u_2} \right] \mathbf{e}_3 \end{aligned} \quad (1.12)$$

3. 几例含哈密顿算符的运算式

3.1. Poisson 方程和 Laplace 方程

标量 ϕ 在正交曲线坐标系 (u_1, u_2, u_3) 连续可微, 存在二阶偏导数, 且矢量 $A = \varepsilon \nabla \phi$ (如电势和电场强度), 那么 $\nabla \cdot A$ 等于什么呢? 将(1.4)式中 3 个分量乘以 ε 代替(1.6)式中的 A_1 、 A_2 、 A_3 有:

$$\nabla \cdot \mathbf{A} = \nabla \cdot \varepsilon \nabla \phi = \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \varepsilon \frac{\partial \phi}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_3 h_1}{h_2} \varepsilon \frac{\partial \phi}{\partial u_2} \right) + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \varepsilon \frac{\partial \phi}{\partial u_3} \right) \right] \quad (2.1)$$

若 $\nabla \cdot \mathbf{A} = f$, 且 $f \neq 0$ 则(2.1)式称 Poisson 方程; 若 $f = 0$ 则称为 Laplace 方程, 令 $\varepsilon = 1$, 可以得到拉普拉斯算符:

$$\nabla^2 = \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial}{\partial u_2} \right) + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial}{\partial u_3} \right) \right] \quad (2.2)$$

3.2. $\nabla \cdot (\mu \mathbf{A}) = (\nabla \mu) \cdot \mathbf{A} + \mu (\nabla \cdot \mathbf{A})$

$\mu(u_1, u_2, u_3)$ 连续可微, 由(1.4)和(1.6)式可得到:

$$\begin{aligned} \nabla \cdot (\mu \mathbf{A}) &= (\nabla \mu) \cdot \mathbf{A} + \mu (\nabla \cdot \mathbf{A}) \\ &= \left[\left(\frac{\partial \mu}{h_1 \partial u_1} \right) A_1 + \left(\frac{\partial \mu}{h_2 \partial u_2} \right) A_2 + \left(\frac{\partial \mu}{h_3 \partial u_3} \right) A_3 \right] \\ &\quad + \frac{\mu}{h_1 h_2 h_3} \left[\frac{\partial}{\partial u_1} (h_2 h_3 A_1) + \frac{\partial}{\partial u_2} (h_3 h_1 A_2) + \frac{\partial}{\partial u_3} (h_1 h_2 A_3) \right] \end{aligned} \quad (2.3)$$

3.3. $\nabla^2 \mathbf{A} = (\nabla^2 A_1) \mathbf{e}_1 + (\nabla^2 A_2) \mathbf{e}_2 + (\nabla^2 A_3) \mathbf{e}_3$

由(2.2)式可得:

$$\begin{aligned} \nabla^2 \mathbf{A} &= (\nabla^2 A_1) \mathbf{e}_1 + (\nabla^2 A_2) \mathbf{e}_2 + (\nabla^2 A_3) \mathbf{e}_3 \\ &= \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial A_1}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial A_1}{\partial u_2} \right) + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial A_1}{\partial u_3} \right) \right] \mathbf{e}_1 \\ &\quad + \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial A_2}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial A_2}{\partial u_2} \right) + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial A_2}{\partial u_3} \right) \right] \mathbf{e}_2 \\ &\quad + \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial A_3}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial A_3}{\partial u_2} \right) + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial A_3}{\partial u_3} \right) \right] \mathbf{e}_3 \end{aligned} \quad (2.4)$$

3.4. $\nabla \times (\nabla \times \mathbf{A}) = \nabla (\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A}$

由(1.4), (1.6), (2.4)三式可以得到

$$\begin{aligned} &\nabla \times (\nabla \times \mathbf{A}) \\ &= \nabla (\nabla \cdot \mathbf{A}) - \nabla^2 \mathbf{A} \\ &= \frac{\partial}{h_1 \partial u_1} \left\{ \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial u_1} (h_1 h_2 A_1) + \frac{\partial}{\partial u_2} (h_3 h_1 A_2) + \frac{\partial}{\partial u_3} (h_1 h_2 A_3) \right] \right\} \mathbf{e}_1 \\ &\quad + \frac{\partial}{h_2 \partial u_2} \left\{ \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial u_1} (h_1 h_2 A_1) + \frac{\partial}{\partial u_2} (h_3 h_1 A_2) + \frac{\partial}{\partial u_3} (h_1 h_2 A_3) \right] \right\} \mathbf{e}_2 \\ &\quad + \frac{\partial}{h_3 \partial u_3} \left\{ \frac{1}{h_1 h_2 h_3} \left[\frac{\partial}{\partial u_1} (h_1 h_2 A_1) + \frac{\partial}{\partial u_2} (h_3 h_1 A_2) + \frac{\partial}{\partial u_3} (h_1 h_2 A_3) \right] \right\} \mathbf{e}_3 \end{aligned}$$

$$\begin{aligned}
& - \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial A_1}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial A_1}{\partial u_2} \right) + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial A_1}{\partial u_3} \right) \right] \mathbf{e}_1 \\
& - \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial A_2}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial A_2}{\partial u_2} \right) + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial A_2}{\partial u_3} \right) \right] \mathbf{e}_2 \\
& - \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial A_3}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial A_3}{\partial u_2} \right) + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial A_3}{\partial u_3} \right) \right] \mathbf{e}_3
\end{aligned} \tag{2.5}$$

3.5. 动量算符 $-i\hbar\nabla$ 与 Schrödinger 方程

由(1.2)式可知动量算符 $-i\hbar\nabla = -i\hbar \left(\mathbf{e}_1 \frac{\partial}{h_1 \partial u_1} + \mathbf{e}_2 \frac{\partial}{h_2 \partial u_2} + \mathbf{e}_3 \frac{\partial}{h_3 \partial u_3} \right)$, 自由粒子波函数 ψ 的波动方程为

$$-i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \left[\frac{\partial}{\partial u_1} \left(\frac{h_2 h_3}{h_1} \frac{\partial \psi}{\partial u_1} \right) + \frac{\partial}{\partial u_2} \left(\frac{h_3 h_1}{h_2} \frac{\partial \psi}{\partial u_2} \right) + \frac{\partial}{\partial u_3} \left(\frac{h_1 h_2}{h_3} \frac{\partial \psi}{\partial u_3} \right) \right] + V(u_1, u_2, u_3) \psi \tag{2.6}$$

4. 在笛卡尔坐标系、柱坐标系和球坐标系的具体形式

4.1. 笛卡尔坐标系

在笛卡尔坐标系中, 坐标因子 $h_1 = 1$, $h_2 = 1$, $h_3 = 1$, $ds_1 = x$, $ds_2 = y$, $ds_3 = z$, 则:

$$\begin{aligned}
\nabla &= \frac{\partial}{\partial s_1} \mathbf{e}_1 + \frac{\partial}{\partial s_2} \mathbf{e}_2 + \frac{\partial}{\partial s_3} \mathbf{e}_3 = \frac{\partial}{\partial x} \mathbf{i} + \frac{\partial}{\partial y} \mathbf{j} + \frac{\partial}{\partial z} \mathbf{k} \\
\nabla \phi &= \left(\frac{\partial \phi}{\partial x} \right) \mathbf{i} + \left(\frac{\partial \phi}{\partial y} \right) \mathbf{j} + \left(\frac{\partial \phi}{\partial z} \right) \mathbf{k} \\
\operatorname{div} \mathbf{A} &= \nabla \cdot \mathbf{A} = \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \\
\operatorname{curl} \mathbf{A} &= \nabla \times \mathbf{A} = \left(\frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) \mathbf{i} + \left(\frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) \mathbf{j} + \left(\frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \mathbf{k} \\
\nabla^2 &= \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}
\end{aligned}$$

4.2. 柱坐标系

在柱坐标系中, 坐标因子 $h_1 = 1$, $h_2 = \rho$, $h_3 = 1$, $ds_1 = d\rho$, $ds_2 = \rho d\varphi$, $ds_3 = dz$ 则:

$$\begin{aligned}
\nabla &= \frac{\partial}{\partial s_1} \mathbf{e}_1 + \frac{\partial}{\partial s_2} \mathbf{e}_2 + \frac{\partial}{\partial s_3} \mathbf{e}_3 = \frac{\partial}{\partial \rho} \mathbf{e}_\rho + \frac{1}{\rho} \frac{\partial}{\partial \varphi} \mathbf{e}_\varphi + \frac{\partial}{\partial z} \mathbf{e}_z \\
\nabla \phi &= \left(\frac{\partial \phi}{\partial \rho} \right) \mathbf{e}_\rho + \frac{1}{\rho} \left(\frac{\partial \phi}{\partial \varphi} \right) \mathbf{e}_\varphi + \left(\frac{\partial \phi}{\partial z} \right) \mathbf{e}_z \\
\operatorname{div} \mathbf{A} &= \nabla \cdot \mathbf{A} = \frac{1}{\rho} \frac{\partial (\rho A_\rho)}{\partial \rho} + \frac{1}{\rho} \frac{\partial A_\varphi}{\partial \varphi} + \frac{\partial A_z}{\partial z} \\
\operatorname{curl} \mathbf{A} &= \nabla \times \mathbf{A} = \left(\frac{1}{\rho} \frac{\partial A_z}{\partial \varphi} - \frac{\partial A_\varphi}{\partial z} \right) \mathbf{e}_\rho + \left(\frac{\partial A_\rho}{\partial z} - \frac{\partial A_z}{\partial \rho} \right) \mathbf{e}_\varphi + \frac{1}{\rho} \left(\frac{\partial (\rho A_\varphi)}{\partial \rho} - \frac{\partial A_\rho}{\partial \varphi} \right) \mathbf{e}_z
\end{aligned}$$

$$\nabla^2 = \frac{1}{\rho} \frac{\partial}{\partial \rho} \left(\rho \frac{\partial}{\partial \rho} \right) + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2}$$

4.3. 球坐标系

球坐标系中, 坐标因子 $h_1 = 1$, $h_2 = r$, $h_3 = r \sin \theta$, $ds_1 = dr$, $ds_2 = r d\theta$, $ds_3 = r \sin \theta d\varphi$, 则:

$$\begin{aligned} \nabla &= \frac{\partial}{\partial r} \mathbf{e}_r + \frac{1}{r} \frac{\partial}{\partial \theta} \mathbf{e}_\theta + \frac{1}{r \sin \theta} \frac{\partial}{\partial \varphi} \mathbf{e}_\varphi \\ \nabla \phi &= \left(\frac{\partial \phi}{\partial r} \right) \mathbf{e}_r + \frac{1}{r} \left(\frac{\partial \phi}{\partial \theta} \right) \mathbf{e}_\theta + \frac{1}{r \sin \theta} \left(\frac{\partial \phi}{\partial \varphi} \right) \mathbf{e}_\varphi \\ \operatorname{div} \mathbf{A} = \nabla \cdot \mathbf{A} &= \frac{1}{r^2} \frac{\partial (r^2 A_r)}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial (A_\theta \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial A_\varphi}{\partial \varphi} \\ \operatorname{curl} \mathbf{A} = \nabla \times \mathbf{A} &= \frac{1}{r \sin \theta} \left(\frac{\partial (A_\varphi \sin \theta)}{\partial \theta} - \frac{\partial A_\theta}{\partial \varphi} \right) \mathbf{e}_r + \frac{1}{r} \left(\frac{1}{\sin \theta} \frac{\partial A_r}{\partial \varphi} - \frac{\partial (r A_\varphi)}{\partial r} \right) \mathbf{e}_\theta + \frac{1}{r} \left(\frac{\partial (r A_\theta)}{\partial r} - \frac{\partial A_r}{\partial \theta} \right) \mathbf{e}_\varphi \\ \nabla^2 &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \end{aligned}$$

5. 结论

通过定义一个三维正交曲线坐标系 (u_1, u_2, u_3) 组成的空间, 以及用 u_1 、 u_2 、 u_3 乘以坐标因子 h_1 、 h_2 、 h_3 来表示三个方向的线长, h_1 、 h_2 、 h_3 是 (u_1, u_2, u_3) 的函数。定义三个线元 $ds_1 = h_1 du_1$, $ds_2 = h_2 du_2$, $ds_3 = h_3 du_3$, 可以得到关于哈密顿算符 ∇ 、 $\nabla \phi$ 、 $\nabla \cdot \mathbf{A}$ 、 $\nabla \times \mathbf{A}$ 、 ∇^2 及的一般表达式 Poisson 方程和 Laplace 方程的一般表达式。在这些表达式中 h_1 、 h_2 、 h_3 取不同的值, 可以演化得到在相应坐标系下的对应运算式。

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