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由含时边界条件的两种有限深量子势阱构造的哈密顿算符和它们的复 BERRY 相位*

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在量子基础理论的框架下分别从一维含时边界条件的半壁无限高量子势阱和三维含时边界条件的有限深球方势阱构造了两种描述带电粒子在电磁场作用下的新哈密顿算符.在绝热近似下,计算了这两种新量子体系的复 Berry 相位.

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1　引　　言

1984 年 Berry[1]通过对绝热定理的重新考察,发现了几何相位,这是量子物理的一个重要进展,引起了人们的广泛研究.Simon[2]立即给予 Berry 相位一拓扑意义,把它看成是复矢量丛的 Holonomy.Wilczek 和 Zee[3]把 Berry 相位由能级非简并情况推广到能级简并情况,得到了 Wilczek-Zee 算符.Aharonov 和 Anandan[4]则仅考察波函数的周期演化情况,而放弃了绝热近似条件,给出一种更广义的几何相位.

近年来,人们对 Berry 相位的研究主要集中在系统的哈密顿算符依赖于时间的含时量子体系上,而不大注意边界条件随时间的变化对量子体系的几何相位所产生的影响.然而人们最近发现含时边界条件对波函数的几何相位也起着重要作用.Levy-LeBlond[5]发现一个传播的量子粒子的空间边界条件区域性的变化将改变波函数的相位.Pereshogen 和 Pronin[6]则讨论了一维含时边界条件的无限深量子势阱,他们用微分几何的方法构造了原哈密顿算符的有效哈密顿算符,然后计算了含时边界条件所导致的体系波函数的 Berry 相位.刘登云[7]在量子基础理论的框架下也构造了一维含时边界条件的无限深量子势阱的有效哈密顿算符,得到了与文献[6]一致的结论.

然而,在文献[6]和[7]中都没有明确指出有效哈密顿算符与原来的哈密顿算符的关系,且他们所研究的体系也较为简单.本文指出文献[6]和[7]中的有效哈密顿算符所描述的量子体系都与一维含时边界的无限深量子势阱不等价.因此文献[6]和[7]中所计算的

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Berry 相位是新量子体系的,它与原来的一维含时边界的无限深量子势阱没有本质联系.然后由两种较具一般性的有限深量子势阱,一个是含时边界条件的一维半壁无限高量子势阱,另一个是含时边界条件的三维有限深球方势阱,用文献[7]的方法在量子基础理论的框架下分别构造了两种描述带电粒子在电磁场作用下的新哈密顿算符.用微扰论的方法计算了新量子体系的瞬时本征态,从而得到了新量子体系波函数的 Berry 相位.结果表明含时边界条件确实导致了波函数的 Berry 相位,且文献[7]中由含时边界条件的一维无限深量子势阱和三维无限深球方势阱构造的新量子体系波函数的 Berry 相位可作为本文的特殊情况而直接得到.

2 文献[6]和[7]中的有效哈密顿算符与原来的哈密顿算符不描写相同体系的理由

在文献[6]和文献[7]中均未明确指出他们构造的有效哈密顿算符所描述的量子体系与原来量子体系是否等价,这样容易使人误认为构造的有效哈密顿算符仍描写原来的量子体系,因而会将文献[6]和[7]中所计算的 Berry 相位当成原来量子体系由于边界条件的变化而产生的几何相位.为避免产生这样的误解,下面给出构造的有效哈密顿算符所描述的量子体系与原量子体系是不等价的理由.

文献[7]指出构造的有效哈密顿算符 $\widehat{H}_{\rm eff}$ 与原哈密顿算符 $\widehat{H}_{(0)}$ 由一静态规范变换 $\mathrm{U}(t)$ 相联系,即

$$\widehat{H}_{\rm eff}=\mathrm{U}(t)\widehat{H}_{(0)}\mathrm{U}(t)^{-1},\quad \mathrm{U}(t)=\exp[\mathrm{i}f(t)]. \tag{1}$$

其中 $f(t)$ 是时间 t 的函数.然而,梁九卿和丁秀香[8]已明确指出由静态规范变换相联系的两个哈密顿算符描述了两个完全不等价的量子体系,规范变换的等价性被破坏.因此文献[6]和[7]中的有效哈密顿算符所描述的量子体系与原量子体系并不等价,他们所计算的 Berry 相位是构造的有效哈密顿算符所描述的量子体系的,而不是原来量子体系的几何相位.文献[6]和[7]实质上是通过一维含时边界的无限深量子势阱用不同的方法构造了一个新量子体系的哈密顿算符,利用原来哈密顿算符的一些结果计算了由含时边界条件导致的新量子体系波函数的 Berry 相位.从另一方面看,由于一维无限深量子势阱的本征函数可取为实数,从而在一维含时边界的无限深量子势阱中的瞬时本征态也可取成实数,因此此体系不可能具有不为零的 Berry 相位.在文献[6]和[7]中选取的量子体系较为简单,且具有一定的局限性.为进一步研究含时边界条件对 Berry 相位的影响,下面我们将由两种含时边界的有限深量子势阱来构造哈密顿算符,得到更普遍的结论.

3 由含时边界的一维半壁无限高势阱构造的量子体系及其复 Berry 相位

设有一个质量为 m 的粒子,被束缚在半壁无限高势阱

$$V(x)=\begin{cases}\infty, & x<0;\\ 0, & 0\leqslant x\leqslant a(t);\\ V_0, & x>a(t)\end{cases}$$

内. 这里 V_0 是大于零的常数, $a(t)$为随时间 t 而变化的边界参数. 显然, 此体系的哈密顿算符为

$$\hat{H}=\begin{cases}\hat{H}_1=\dfrac{\hat{P}^2}{2m}, & 0\leqslant x\leqslant a(t);\\ \hat{H}_2=\dfrac{\hat{P}^2}{2m}+V_0, & x>a(t).\end{cases}\tag{2}$$

由上述体系的瞬时能量本征方程

$$\hat{H}|\phi_n\rangle=E_n|\phi_n\rangle,$$

即

$$\begin{aligned}&\hat{H}_1|\phi_{1n}\rangle=E_n|\phi_{1n}\rangle, && 0\leqslant x\leqslant a(t);\\ &\hat{H}_2|\phi_{2n}\rangle=E_n|\phi_{2n}\rangle, && x>a(t).\end{aligned}\tag{3}$$

不难得到本征能量 E_n 满足超越方程

$$k_{1n}\cos(k_{1n}a)=-k_{2n}\sin(k_{1n}a).\tag{4}$$

这里 $k_{1n}=\left(\dfrac{2mE_n}{\hbar^2}\right)^{1/2}$, $k_{2n}=\left[\dfrac{2m(V_0-E_n)}{\hbar^2}\right]^{1/2}$. 由图解法可知本征能量为一系列分立值且为 $a(t)$的函数. 而此体系的归一化的瞬时能量本征态为

$$|\phi_n\rangle=\begin{cases}|\phi_{1n}\rangle=A_n(a)\sin(k_{1n}x)\exp\left[-\dfrac{i}{\hbar}\displaystyle\int_0^t E_n(a(t'))dt'\right], & 0\leqslant x\leqslant a(t);\\ |\phi_{2n}\rangle=B_n(a)\exp[-k_{2n}x]\exp\left[-\dfrac{i}{\hbar}\displaystyle\int_0^t E_n(a(t'))dt'\right], & x>a(t),\end{cases}\tag{5}$$

其中

$$A_n(a)=\left(\frac{2k_{2n}}{1+ak_{2n}}\right)^{1/2},\tag{6}$$

$$B_n(a)=\left(\frac{2k_{2n}}{1+ak_{2n}}\right)^{1/2}\sin(k_{1n}a)\exp[k_{2n}a].\tag{7}$$

下面我们将应用文献[7]中的方法, 在量子基础理论的框架下构造新的哈密顿算符. 用算符 $i\hbar\dfrac{\partial}{\partial t}$作用于(5)式, 计算表明

$$i\hbar\frac{\partial}{\partial t}|\phi_n\rangle=\begin{cases}[E_n(a)+i\hbar\dot{a}\nabla_a\ln A_n+i\hbar\dot{a}(\nabla_a\ln k_{1n})x\nabla_x]|\phi_{1n}\rangle, & 0\leqslant x\leqslant a(t);\\ [E_n(a)+i\hbar\dot{a}\nabla_a\ln B_n+i\hbar\dot{a}(\nabla_a\ln k_{2n})x\nabla_x]|\phi_{2n}\rangle, & x>a(t).\end{cases}\tag{8}$$

将上式视为以$|\phi_n\rangle$为波函数的含时 Schrödinger 方程, 结合本征方程(3)式, 得到新量子体系的哈密顿算符

$$\hat{H}' = \begin{cases} \hat{H}_1' = \hat{H}_1 + \mathrm{i}\hbar\dot{a}\left[\nabla_a \ln A_n + (\nabla_a \ln k_{1n}) x \nabla_x\right], & 0 \leqslant x \leqslant a(t); \\ \hat{H}_2' = \hat{H}_2 + \mathrm{i}\hbar\dot{a}\left[\nabla_a \ln B_n + (\nabla_a \ln k_{2n}) x \nabla_x\right], & x > a(t). \end{cases} \tag{9}$$

将$\frac{\partial}{\partial a}$作用于(4)式两边，并利用 $k_{1n}^2 + k_{2n}^2 = \frac{2mV_0}{\hbar^2}$，可得

$$\frac{\partial k_{1n}}{\partial a} = -\frac{k_{1n}k_{2n}}{1 + ak_{2n}}, \quad \frac{\partial k_{2n}}{\partial a} = -\frac{k_{1n}}{k_{2n}}\frac{\partial k_{1n}}{\partial a} = \frac{k_{1n}^2}{1 + ak_{2n}}. \tag{10}$$

再由(6)和(7)式，得

$$\nabla_a \ln A_n = \frac{1}{2k_{2n}(1 + ak_{2n})}\frac{\partial k_{2n}}{\partial a} - \frac{k_{2n}}{2(1 + ak_{2n})}, \tag{11}$$

$$\nabla_a \ln B_n = \nabla_a \ln A_n + \left(k_{1n} + a\frac{\partial k_{1n}}{\partial a}\right)\cot(k_{1n}a) + k_{2n} - \frac{ak_{1n}}{k_{2n}}\frac{\partial k_{1n}}{\partial a}. \tag{12}$$

将(10)，(11)和(12)式代入(9)式并利用算符关系 $x\frac{\partial}{\partial x} - \frac{\partial}{\partial x}x = -1$，易得

$$\hat{H}' = \begin{cases} \hat{H}_1' = \hat{H}_1 + \mathrm{i}\hbar\dot{a}\frac{1}{2k_{1n}}\frac{\partial k_{1n}}{\partial a}(\nabla_x x + x\nabla_x) + \mathrm{i}\hbar\dot{a}\frac{k_{1n}^2}{2k_{2n}(1 + ak_{2n})^2}, \\ \hat{H}_2' = \hat{H}_2 + \mathrm{i}\hbar\dot{a}\frac{1}{2k_{2n}}\frac{\partial k_{2n}}{\partial a}(\nabla_x x + x\nabla_x) \\ \qquad + \mathrm{i}\hbar\dot{a}\left[\frac{-k_{2n}^2}{2(1 + ak_{2n})^2} + \frac{a(k_{1n}^2 + k_{2n}^2)(1 + 2ak_{2n})}{2(1 + ak_{2n})^2}\right]. \end{cases} \tag{13}$$

设 c 表示光速，q 为粒子的电荷，令

$$\mathscr{A}_1 = \frac{mc\dot{a}}{qk_{1n}}\frac{\partial k_{1n}}{\partial a}x, \quad \varphi_1 = \mathrm{i}\hbar\frac{\dot{a}}{q}\frac{k_{1n}^2}{2k_{2n}(1 + ak_{2n})^2};$$

$$\mathscr{A}_2 = \frac{mc\dot{a}}{qk_{2n}}\frac{\partial k_{2n}}{\partial a}x, \quad \varphi_2 = \mathrm{i}\hbar\frac{\dot{a}}{q}\left[\frac{-k_{2n}^2}{2(1 + ak_{2n})^2} + \frac{a(k_{1n}^2 + k_{2n}^2)(1 + 2ak_{2n})}{2(1 + ak_{2n})^2}\right].$$

代入(13)式得

$$\hat{H}' = \begin{cases} \hat{H}_1' \doteq \frac{1}{2m}\left(\hat{P}_x - \frac{q}{c}\mathscr{A}_1\right)^2 + q\varphi_1, & 0 \leqslant x \leqslant a(t); \\ \hat{H}_2' \doteq \frac{1}{2m}\left(\hat{P}_x - \frac{q}{c}\mathscr{A}_2\right)^2 + q\varphi_2 + V_0, & x > a(t). \end{cases} \tag{14}$$

在这里，为满足绝热定理所要求的条件，我们已让 $a(t)$做缓慢变化，从而忽略了 $\dot{a}(t)$的二次项.(14)式就是我们从含时边界的一维半壁无限高量子势阱构造的哈密顿算符，它所描述的量子体系与一维半壁无限高量子势阱并不等价.实质上它描写了一个质量为 m 电荷为 q 的粒子在电磁场作用下的新量子体系.此电磁场在 $0 \leqslant x \leqslant a(t)$区域是由矢势 $\mathscr{A}_1$ 和标势 φ_1 产生的，而在 $x > a(t)$区域则由矢势 $\mathscr{A}_2$ 和标势 $\varphi_2 + \frac{V_0}{q}$形成的.此新哈密顿算符的另一特点是标势 φ_1 和标势 φ_2 为随时间变化的纯虚数，因而 $\hat{H}'$不再是厄米算符.它适合描述耗散、弛豫等开系统的量子过程.关于非厄米哈密顿算符的量子力学人们已做了广泛深入的研究，并得到了 Berry 相位的计算公式[9,10].Dattoli 等[9]证明，在哈密顿算

符 $\hat{H}$ 为非厄米算符时, $\hat{H}$ 和 $\hat{H}^\dagger$ 的本征方程

$$\hat{H}|\varphi_n\rangle = \varepsilon_n|\varphi_n\rangle; \quad \hat{H}^\dagger|\chi_m\rangle = \varepsilon_m^*|\chi_m\rangle \tag{15}$$

的解 $|\varphi_n\rangle$ 和 $|\chi_m\rangle$ 是满足下面关系

$$\langle\chi_m|\varphi_n\rangle = \langle\varphi_n|\chi_m\rangle = \delta_{mn}; \tag{16}$$

$$\sum_n|\varphi_n\rangle\langle\chi_n| = \sum_n|\chi_n\rangle\langle\varphi_n| = 1 \tag{17}$$

的双正交归一化基矢. 瞬时本征态 $|\varphi_n\rangle$ 和 $|\chi_n\rangle$ 的复 Berry 相位的计算公式为

$$\gamma_c = \mathrm{i}\int_0^T\langle\chi_n|\frac{\partial}{\partial t}|\varphi_n\rangle\mathrm{d}t. \tag{18}$$

下面我们将用微扰论的方法找出新哈密顿算符的一个瞬时本征态, 然后计算出此本征态的复 Berry 相位. 设 $\hat{H}'$ 的瞬时本征方程为

$$\hat{H}'|\phi_m'\rangle = E_m'|\phi_m'\rangle,$$

即

$$\begin{aligned}&\hat{H}_1'|\phi_{1m}'\rangle = E_m'|\phi_{1m}'\rangle, \quad 0\leqslant x\leqslant a(t);\\&\hat{H}_2'|\phi_{2m}'\rangle = E_m'|\phi_{2m}'\rangle, \quad x > a(t).\end{aligned} \tag{19}$$

对上式做变换, 令

$$\hat{\mathscr{H}} = \hat{U}_1^\dagger\hat{H}'\hat{U}_1, \tag{20}$$

其中 $\hat{U}_1 = \exp[\mathrm{i}f_1(t)]$, $f_1(t) = \frac{q}{\hbar c}\int\mathscr{A}_1\mathrm{d}x = \frac{m\dot{a}}{2\hbar k_{1n}}\frac{\partial k_{1n}}{\partial a}x^2$. 显然知道了 $\hat{\mathscr{H}}$ 的瞬时能量本征态, 则可求得 $\hat{H}'$ 的瞬时能量本征态, 因此我们首先研究 $\hat{\mathscr{H}}$ 的瞬时能量本征方程

$$\hat{\mathscr{H}}|\Phi_m\rangle = E_m'|\Phi_m\rangle \tag{21}$$

的解, 而 $|\Phi_m\rangle = \hat{U}_1^\dagger|\phi_m'\rangle$. 将 $\hat{H}'$ 的表示式(14)代入(20)式, 并利用公式

$$\mathrm{e}^{\hat{L}}\hat{A}\mathrm{e}^{-\hat{L}} = \hat{A} + [\hat{L},\hat{A}] + \frac{1}{2!}[\hat{L},[\hat{L},\hat{A}]] + \cdots, \tag{22}$$

且忽略 $\dot{a}(t)$ 的二次以上项, 整理可得

$$\hat{\mathscr{H}} = \begin{cases}\hat{\mathscr{H}}_1 = \hat{H}_1 + q\varphi_1, & 0\leqslant x\leqslant a(t);\\ \hat{\mathscr{H}}_2 = \hat{H}_2 + q\varphi_1 + \mathrm{i}\hbar\dot{a}\left[\frac{k_{1n}^2+k_{2n}^2}{k_{2n}(1+ak_{2n})}x\frac{\partial}{\partial x} + \frac{a(k_{1n}^2+k_{2n}^2)}{1+ak_{2n}}\right], & x > a(t).\end{cases} \tag{23}$$

当 $a(t)$ 缓慢变化时, 可将上式中的

$$\hat{\mathscr{H}}' = \begin{cases}0, & 0\leqslant x\leqslant a(t);\\ \mathrm{i}\hbar\dot{a}\frac{k_{1n}^2+k_{2n}^2}{1+ak_{2n}}\left(\frac{1}{k_{2n}}x\frac{\partial}{\partial x}+a\right), & x > a(t)\end{cases}$$

视为

$$\hat{\mathscr{H}}_0 = \begin{cases}\hat{H}_1 + q\varphi_1, & 0\leqslant x\leqslant a(t);\\ \hat{H}_2 + q\varphi_1, & x > a(t)\end{cases}$$

的微扰.不难看出$\hat{\mathscr{H}}_0$的瞬时本征方程的解即为方程(3)的解,已经求得.将对应于$\hat{\mathscr{H}}_0$的能量本征值为$E_n+q\varphi_1$取为零级近似$E_n'^{(0)}$,由普通微扰论[11]容易得到非厄米哈密顿算符$\hat{\mathscr{H}}$的瞬时本征方程准确到一阶的解为(其他情况的本征态解我们将在别处讨论)

$$E_n' = E_n'^{(0)} + E_n'^{(1)}; \qquad |\Phi_n\rangle = |\Phi_n^{(0)}\rangle + |\Phi_n^{(1)}\rangle, \tag{24}$$

其中

$$E_n'^{(0)} = E_n + q\varphi_1, \tag{25}$$

$$|\Phi_n^{(0)}\rangle = |\chi_n^{(0)}\rangle = |\phi_n\rangle, \tag{26}$$

$$\begin{aligned} E_n'^{(1)} &= \langle \chi_n^{(0)} | \hat{\mathscr{H}}' | \Phi_n^{(0)} \rangle \\ &= -\mathrm{i}\hbar\dot{a}\frac{(k_{1n}^2 + k_{2n}^2)\sin^2(k_{1n}a)}{2k_{2n}(1+ak_{2n})^2}, \end{aligned} \tag{27}$$

$$\begin{aligned} |\Phi_n^{(1)}\rangle &= \sum_{m\neq n}\frac{\langle \chi_m^{(0)} | \hat{\mathscr{H}}' | \Phi_n^{(0)} \rangle}{E_n - E_m}|\Phi_m^{(0)}\rangle \\ &= -2\mathrm{i}\hbar\dot{a}\frac{k_{1n}^2 + k_{2n}^2}{1+ak_{2n}}\left(\frac{k_{2n}}{1+ak_{2n}}\right)^{1/2}\sin(k_{1n}a) \\ &\quad\times\sum_{m\neq n}\frac{(k_{2m})^{1/2}\sin(k_{1m}a)}{(E_n - E_m)(1+ak_{2m})^{1/2}(k_{2n}+k_{2m})^2}|\phi_m\rangle. \end{aligned} \tag{28}$$

由此得到$\hat{H}'$的瞬时能量本征态为

$$|\phi_n'\rangle = \hat{U}_1|\Phi_n\rangle = \hat{U}_1(|\Phi_n^{(0)}\rangle + |\Phi_n^{(1)}\rangle). \tag{29}$$

同理可求出$\hat{\mathscr{H}}^\dagger$的瞬时能量本征方程的微扰展开解为

$$\begin{aligned} E_n'^{*} &= E_n'^{(0)*} + E_n'^{(1)*} \\ &= E_n - \mathrm{i}\hbar\dot{a}\frac{k_{1n}^2 - (k_{1n}^2 + k_{2n}^2)\sin^2(k_{1n}a)}{2k_{2n}(1+ak_{2n})^2}, \end{aligned} \tag{30}$$

$$\begin{aligned} \langle \chi_n| &= \langle \chi_n^{(0)}| + \langle \chi_n^{(1)}| \\ &= \langle \Phi_n^{(0)}| + \langle \Phi_n^{(1)}| \\ &= \langle \phi_n| + 2\mathrm{i}\hbar\dot{a}\frac{k_{1n}^2 + k_{2n}^2}{1+ak_{2n}}\left(\frac{k_{2n}}{1+ak_{2n}}\right)^{1/2}\sin(k_{1n}a) \\ &\quad\times\sum_{m\neq n}\frac{(k_{2m})^{1/2}\sin(k_{1m}a)}{(E_n - E_m)(1+ak_{2m})^{1/2}(k_{2n}+k_{2m})^2}\langle \phi_m|. \end{aligned} \tag{31}$$

由此得$\hat{H}'^\dagger$的瞬时能量本征态

$$\langle \chi_n'| = \langle \chi_n|\hat{U}_1^\dagger = (\langle \Phi_n^{(0)}| + \langle \Phi_n^{(1)}|)\hat{U}_1^\dagger. \tag{32}$$

设$a(t)$做缓慢的周期变化,由$\hat{H}'$所确定的波函数经过一个周期T的时间演化后,其动力学相位为

$$-\frac{\mathrm{i}}{\hbar}\int_0^T E_n'\mathrm{d}t = -\frac{\mathrm{i}}{\hbar}\int_0^T\left[E_n + \mathrm{i}\hbar\dot{a}\frac{k_{1n}^2 - (k_{1n}^2 + k_{2n}^2)\sin^2(k_{1n}a)}{2k_{2n}(1+ak_{2n})^2}\right]\mathrm{d}t. \tag{33}$$

按(18)式,并利用(29)和(32)两式,且注意到$\langle \phi_m | \phi_n \rangle = \delta_{mn}$,可求得此波函数的复 Berry 相位为

$$\gamma_c = -\int_0^T \langle \phi_n | \left(\frac{\partial}{\partial t} f_1 \right) | \phi_n \rangle \mathrm{d}t + 2\mathrm{i} \int_0^T \langle \phi_n | \left(\frac{\partial}{\partial t} | \Phi_n^{(1)} \rangle \right) \mathrm{d}t + \mathrm{i} \int_0^T \langle \chi_n^{(1)} | \hat{U}_1^\dagger \frac{\partial}{\partial t} (\hat{U}_1 | \Phi_n^{(1)} \rangle) \mathrm{d}t, \tag{34}$$

其中

$$-\int_0^T \langle \phi_n | \left(\frac{\partial}{\partial t} f_1 \right) | \phi_n \rangle \mathrm{d}t = \int_0^T \left[\frac{a^3}{6} + \frac{1 - 2a^2 k_{1n}^2}{8 k_{1n}^3} \sin(2k_{1n}a) - \frac{a}{4k_{1n}^2} \cos(2k_{1n}a) + \frac{2a^2 k_{2n}^2 + 2ak_{2n} + 1}{4k_{2n}^3} \sin^2(k_{1n}a) \right] \times \frac{2k_{2n}}{1 + ak_{2n}} \left[\frac{mk_{2n}}{2\hbar(1 + ak_{2n})} \mathrm{d}\dot{a} + \frac{m\dot{a}}{2\hbar} \mathrm{d} \left(\frac{k_{2n}}{1 + ak_{2n}} \right) \right], \tag{35}$$

$$2\mathrm{i} \int_0^T \langle \phi_n | \left(\frac{\partial}{\partial t} | \Phi_n^{(1)} \rangle \right) \mathrm{d}t = 4\hbar \int_0^T \frac{k_{1n}^2 + k_{2n}^2}{1 + ak_{2n}} \left(\frac{k_{2n}}{1 + ak_{2n}} \right)^{1/2} \sin(k_{1n}a) \times \sum_{m \neq n} \frac{(k_{2m})^{1/2} \sin(k_{1m}a)}{(E_n - E_m)(1 + ak_{2m})^{1/2}(k_{2n} + k_{2m})^2} \times \langle \phi_n | \left(\frac{\partial}{\partial t} | \phi_m \rangle \right) \mathrm{d}a, \tag{36}$$

而(36)式中的

$$\langle \phi_n | \left(\frac{\partial}{\partial t} | \phi_m \rangle \right) = \left[\frac{4k_{2n}k_{2m}}{(1 + ak_{2n})(1 + ak_{2m})} \right]^{1/2} \dot{a} \times \left\{ \frac{\sin(k_{1n}a)}{k_{2n} + k_{2m}} \left[\cos(k_{1m}a) \left(a \frac{\partial k_{1m}}{\partial a} + k_{1m} \right) + \sin(k_{1m}a) \left(k_{2m} - \frac{1}{k_{2n} + k_{2m}} \frac{\partial k_{2m}}{\partial a} \right) \right] + \left[\frac{\sin(k_{1n} + k_{1m})a}{(k_{1n} + k_{1m})^2} - \frac{a\cos(k_{1n} + k_{1m})a}{k_{1n} + k_{1m}} + \frac{\sin(k_{1n} - k_{1m})a}{(k_{1n} - k_{1m})^2} - \frac{a\cos(k_{1n} - k_{1m})a}{k_{1n} - k_{1m}} \right] \frac{\partial k_{1m}}{\partial a} \right\},$$

$$\mathrm{i} \int_0^T \langle \chi_n^{(1)} | \hat{U}_1^\dagger \frac{\partial}{\partial t} (\hat{U}_1 | \Phi_n^{(1)} \rangle) \mathrm{d}t \doteq 4\mathrm{i}\hbar^2 \int_0^T \frac{k_{2n}(k_{1n}^2 + k_{2n}^2)^2}{(1 + ak_{2n})^3} \sin^2(k_{1n}a) \times \sum_{m \neq n} \frac{k_{2m} \sin^2(k_{1m}a)}{(E_n - E_m)^2 (1 + ak_{2m})(k_{2n} + k_{2m})^4} \dot{a} \mathrm{d}\dot{a}. \tag{37}$$

上式中我们已忽略了 $\dot{a}(t)$的二次以上项.

在 $V_0 \to \infty$ 的极限情况下,$k_{2n} = \left[\frac{2m(V_0 - E_n)}{\hbar^2} \right]^{1/2}$ 也趋于∞. 此时由(4)式可知

$k_{1n}=\frac{n\pi}{a}$, 因此有 $\sin(k_{1n}a)=0$, $\cos(k_{1n}a)=1$. 因此容易看出(36)和(37)两式均为0, 故此时的 Berry 相位为

$$\gamma_c=\frac{m}{2\hbar}\left(\frac{1}{3}-\frac{1}{2n^2\pi^2}\right)\int_0^T[-\dot{a}\,\mathrm{d}a+a\,\mathrm{d}\dot{a}]. \tag{38}$$

如果我们选取 $a(t)=a_0+a_0'\sin\varphi(t)$ 且 $\alpha=\dot{\varphi}=\mathrm{const.}$, 则可得

$$\gamma_c=-\frac{m}{\hbar}\left(\frac{1}{3}-\frac{1}{2n^2\pi^2}\right)a_0'^2\alpha\pi. \tag{39}$$

这与文献[7]的结果完全一致, 因此文献[7]的结论是本文结论的一个特殊情况.

4 由含时边界的三维有限深球方势阱构造的量子体系及其复 Berry 相位

三维有限深球方势阱的势场为

$$V(r)=\begin{cases}0, & 0\leqslant r\leqslant a(t);\\ V_0, & r>a(t).\end{cases}$$

这里 V_0 是大于零的常数, r 是球坐标系中的径向坐标, $a(t)$ 为随时间 t 变化的边界参数. 在此势场中, 质量为 m 的粒子的径向哈密顿算符为

$$\hat{H}_r=\begin{cases}\hat{H}_{r1}=\dfrac{\hat{P}_r^2}{2m}+\dfrac{l(l+1)\hbar^2}{2mr^2}, & 0\leqslant r\leqslant a(t);\\[2ex] \hat{H}_{r2}=\dfrac{\hat{P}_r^2}{2m}+\dfrac{l(l+1)\hbar^2}{2mr^2}+V_0, & r>a(t).\end{cases} \tag{40}$$

其中 $\hat{P}_r=-\mathrm{i}\hbar\frac{1}{r}\frac{\partial}{\partial r}r$ 为径向动量算符, l 是对应的角动量量子数. 由上述体系的径向瞬时能量本征方程

$$\hat{H}_r|R\rangle=E|R\rangle,$$

即

$$\begin{aligned}&\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R_1}{\mathrm{d}r}\right)+\left[\frac{2m}{\hbar^2}E-\frac{l(l+1)}{r^2}\right]R_1=0, \quad 0\leqslant r\leqslant a(t);\\ &\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}R_2}{\mathrm{d}r}\right)+\left[\frac{2\mathrm{i}^2m}{\hbar^2}(V_0-E)-\frac{l(l+1)}{r^2}\right]R_2=0, \quad r>a(t),\end{aligned} \tag{41}$$

根据特殊函数理论[12], 并利用球贝塞尔函数 j_l 和虚宗量球汉克耳函数 h_l 所遵从的相同递推关系

$$j_l'(x)=j_{l-1}(x)-\frac{l+1}{x}j_l(x); \quad j_l'(x)=-j_{l+1}(x)+\frac{l}{x}j_l(x), \tag{42}$$

不难得到本征能量 E 所满足的超越方程

$$k_1\frac{j_{l-1}(k_1a)}{j_l(k_1a)}=\mathrm{i}k_2\frac{h_{l-1}^{(1)}(\mathrm{i}k_2a)}{h_l^{(1)}(\mathrm{i}k_2a)}, \tag{43}$$

这里 $k_1=\left(\frac{2mE}{\hbar^2}\right)^{1/2}$, $k_2=\left[\frac{2m(V_0-E)}{\hbar^2}\right]^{1/2}$. 由此方程可得一系列的分立能量本征值,不妨将与序号 n 对应的本征能量取成 $E_{l,n}(a(t))$. 当角动量量子数 l 为偶数时,$h_l^{(1)}(\mathrm{i}k_2r)$为实数,当 l 为奇数时,$h_l^{(1)}(\mathrm{i}k_2r)$为纯虚数. 为简单起见,我们只考虑 l 为偶数时的情况,并令 $h_l(\mathrm{i}k_2r)=h_l^{(1)}(\mathrm{i}k_2r)$,且将 k_1, k_2 分别记为 k_{1n}, k_{2n}. 而此体系的归一化瞬时能量本征态为

$$|R_n(r,a(t))\rangle=\begin{cases}|R_{1n}\rangle = A_{l,n}j_l(k_{1n}r)\exp\left[-\frac{\mathrm{i}}{\hbar}\int_0^t E_{l,n}(a(t'))\mathrm{d}t'\right], & 0\leqslant r\leqslant a(t);\\ |R_{2n}\rangle = B_{l,n}h_l(\mathrm{i}k_{2n}r)\exp\left[-\frac{\mathrm{i}}{\hbar}\int_0^t E_{l,n}(a(t'))\mathrm{d}t'\right], & r>a(t),\end{cases}\tag{44}$$

其中

$$A_{l,n}=\left[-\frac{(k_{1n}^2+k_{2n}^2)a^3}{2k_{2n}^2}j_{l-1}(k_{1n}a)j_{l+1}(k_{1n}a)\right]^{-1/2},\tag{45}$$

$$B_{l,n}=\frac{j_l(k_{1n}a)}{h_l(\mathrm{i}k_{2n}a)}\left[-\frac{(k_{1n}^2+k_{2n}^2)a^3}{2k_{2n}^2}j_{l-1}(k_{1n}a)j_{l+1}(k_{1n}a)\right]^{-1/2}.\tag{46}$$

下面从(44)式所给出的瞬时能量本征态出发,构造新量子体系的哈密顿算符. 将算符 $\mathrm{i}\hbar\frac{\partial}{\partial t}$作用到(44)式,计算表明

$$\mathrm{i}\hbar\frac{\partial}{\partial t}|R_n(r,a(t))\rangle=\begin{cases}[E_{l,n}(a)+\mathrm{i}\hbar\dot{a}\nabla_a\ln A_{l,n}+\mathrm{i}\hbar\dot{a}(\nabla_a\ln k_{1n})r\nabla_r]|R_{1n}\rangle, & 0\leqslant r\leqslant a(t);\\ [E_{l,n}(a)+\mathrm{i}\hbar\dot{a}\nabla_a\ln B_{l,n}+\mathrm{i}\hbar\dot{a}(\nabla_a\ln k_{2n})r\nabla_r]|R_{2n}\rangle, & x>a(t).\end{cases}\tag{47}$$

将上式视为以$|R_n\rangle$为波函数的含时 Schrödinger 方程,结合本征方程(41)式,得到新量子体系的哈密顿算符

$$\hat{H}_r'=\begin{cases}\hat{H}_{r1}'=\hat{H}_{r1}+\mathrm{i}\hbar\dot{a}[\nabla_a\ln A_{l,n}+(\nabla_a\ln k_{1n})r\nabla_r], & 0\leqslant r\leqslant a(t);\\ \hat{H}_{r2}'=\hat{H}_{r2}+\mathrm{i}\hbar\dot{a}[\nabla_a\ln B_{l,n}+(\nabla_a\ln k_{2n})r\nabla_r], & r>a(t).\end{cases}\tag{48}$$

(43)式两边用$\frac{\partial}{\partial a}$作用,并利用(42)和(43)两式,可得

$$\frac{\partial k_{1n}}{\partial a}=\frac{j_l^2k_{2n}^2}{ak_{1n}j_{l+1}j_{l-1}};\quad \frac{\partial k_{2n}}{\partial a}=-\frac{k_{1n}}{k_{2n}}\frac{\partial k_{1n}}{\partial a}=-\frac{j_l^2k_{2n}}{aj_{l+1}j_{l-1}}.\tag{49}$$

这里的 $j_l=j_l(k_{1n}a)$. 再由 $A_{l,n}$和 $B_{l,n}$的表达式(45)和(46),计算得

$$\nabla_a\ln A_{l,n}=\left(\frac{k_{1n}}{k_{2n}^2}-\frac{3}{2k_{1n}}\right)\frac{\partial k_{1n}}{\partial a}+\frac{1}{2}\left(k_{1n}+a\frac{\partial k_{1n}}{\partial a}\right)\left(\frac{1}{j_{l+1}}-\frac{1}{j_{l-1}}\right)j_l,\tag{50}$$

$$\nabla_a\ln B_{l,n}=\nabla_a\ln A_{l,n}+\frac{k_{1n}^2+k_{2n}^2}{k_{1n}k_{2n}}\frac{\partial k_{1n}}{\partial a}\left(\mathrm{i}a\frac{h_{l-1}}{h_l}-\frac{l+1}{k_{2n}}\right).\tag{51}$$

这里的 $h_l=h_l(\mathrm{i}k_{2n}a)$.利用算符的对易关系$\frac{\partial}{\partial r}r-r\frac{\partial}{\partial r}=1$,整理(48)式得

$$\hat{H}_r'=\begin{cases}\hat{H}_{r1}'=\hat{H}_{r1}+\mathrm{i}\hbar\dot{a}\dfrac{1}{2k_{1n}}\dfrac{\partial k_{1n}}{\partial a}\left(\dfrac{\partial}{\partial r}r+r\dfrac{\partial}{\partial r}\right)+\mathrm{i}\hbar\dot{a}\left(\nabla_a\ln A_{l,n}-\dfrac{1}{2k_{1n}}\dfrac{\partial k_{1n}}{\partial a}\right),\\ \hat{H}_{r2}'=\hat{H}_{r2}+\mathrm{i}\hbar\dot{a}\dfrac{1}{2k_{2n}}\dfrac{\partial k_{2n}}{\partial a}\left(\dfrac{\partial}{\partial r}r+r\dfrac{\partial}{\partial r}\right)+\mathrm{i}\hbar\dot{a}\left(\nabla_a\ln B_{l,n}-\dfrac{1}{2k_{2n}}\dfrac{\partial k_{2n}}{\partial a}\right).\end{cases}\tag{52}$$

令

$$\mathscr{A}_1'=\frac{mc\dot{a}}{qk_{1n}}\frac{\partial k_{1n}}{\partial a}r,\qquad \varphi_1'=\mathrm{i}\hbar\frac{\dot{a}}{q}\left(\nabla_a\ln A_{l,n}-\frac{3}{2k_{1n}}\frac{\partial k_{1n}}{\partial a}\right);$$

$$\mathscr{A}_2'=\frac{mc\dot{a}}{qk_{2n}}\frac{\partial k_{2n}}{\partial a}r,\qquad \varphi_2'=\mathrm{i}\hbar\frac{\dot{a}}{q}\left(\nabla_a\ln B_{l,n}-\frac{3}{2k_{2n}}\frac{\partial k_{2n}}{\partial a}\right),$$

代入(52)式,并结合 $\hat{P}_r=-\mathrm{i}\hbar\frac{1}{r}\frac{\partial}{\partial r}r$,得

$$\hat{H}_r'=\begin{cases}\hat{H}_{r1}'\doteq\dfrac{1}{2m}\left(\hat{P}_r-\dfrac{q}{c}\mathscr{A}_1'\right)^2+q\varphi_1'+\dfrac{l(l+1)\hbar^2}{2mr^2}, & 0\leqslant r\leqslant a(t);\\ \hat{H}_{r2}'\doteq\dfrac{1}{2m}\left(\hat{P}_r-\dfrac{q}{c}\mathscr{A}_2'\right)^2+q\varphi_2'+V_0+\dfrac{l(l+1)\hbar^2}{2mr^2}, & r>a(t).\end{cases}\tag{53}$$

在这里,我们让 $a(t)$缓慢变化,因此忽略了 $\dot{a}(t)$的二次项.上式就是我们从三维有限深球方势阱构造的哈密顿算符.容易看出,它实质上描写了一个质量为 m 电荷为 q 的粒子在电磁场作用下的新量子体系.此电磁场在$0\leqslant r\leqslant a(t)$区域是由矢势 $\mathscr{A}_1'$和标势 φ_1' 产生的,而在 $r>a(t)$的区域则由矢势 $\mathscr{A}_2'$和标势 $\varphi_2'+\frac{V_0}{q}$形成的.由于标势 φ_1' 和 φ_2' 也是随时间变化的纯虚数,因而 $\hat{H}_r'$是非厄米算符.我们将仿照上节所用的方法求解 $\hat{H}_r'$的一个瞬时能量本征态,然后计算出此本征态的复 Berry 相位.设 $\hat{H}_r'$ 的瞬时本征方程为

$$\hat{H}_r'|R_m'\rangle=E_{l,m}'|R_m'\rangle,$$

即

$$\begin{cases}\hat{H}_{r1}'|R_{1m}'\rangle=E_{l,m}'|R_{1m}'\rangle, & 0\leqslant r\leqslant a(t);\\ \hat{H}_{r2}'|R_{2m}'\rangle=E_{l,m}'|R_{2m}'\rangle, & r>a(t).\end{cases}\tag{54}$$

为求得上述方程的解,我们对上式做变换,令

$$\hat{\mathscr{H}}_r=\hat{U}_2^{\dagger}\hat{H}_r'\hat{U}_2,\tag{55}$$

其中 $\hat{U}_2=\exp[\mathrm{i}f_2(t)]$, $f_2(t)=\frac{q}{\hbar c}\int\mathscr{A}_1'\mathrm{d}r=\frac{m\dot{a}}{2\hbar k_{1n}}\frac{\partial k_{1n}}{\partial a}r^2$.因此求出了$\hat{\mathscr{H}}_r$的瞬时能量本征态,就可得到 $\hat{H}_r'$ 的瞬时能量本征态.下面我们首先研究$\hat{\mathscr{H}}_r$的瞬时能量本征方程

$$\hat{\mathscr{H}}_r|\mathscr{R}_m\rangle=E_{l,m}'|\mathscr{R}_m\rangle\tag{56}$$

的解,而$|\mathscr{R}_m\rangle=\hat{U}_2^{\dagger}|R_m'\rangle$.将 $\hat{H}_r'$ 的表示式(53)代入(55)式,并利用(22)式,且忽略 $\dot{a}(t)$的二次以上项,整理可得

$$\hat{\mathscr{H}}_r = \begin{cases} \hat{\mathscr{H}}_{r1} = \hat{\mathrm{H}}_{r1} + q\varphi_1', & 0 \leqslant r \leqslant a(t); \\ \hat{\mathscr{H}}_{r2} = \hat{\mathrm{H}}_{r2} + q\varphi_1' - \mathrm{i}\hbar\dot{a}\dfrac{k_{1n}^2 + k_{2n}^2}{k_{1n}k_{2n}}\dfrac{\partial k_{1n}}{\partial a}\left[\dfrac{1}{k_{2n}}\dfrac{\partial}{\partial r}r - \mathrm{i}a\dfrac{h_{l-1}}{h_l} + \dfrac{l}{k_{2n}}\right], & r > a(t). \end{cases} \tag{57}$$

当 $a(t)$缓慢变化时,可将上式中的

$$\hat{\mathscr{H}}_r' = \begin{cases} 0, & 0 \leqslant r \leqslant a(t); \\ -\mathrm{i}\hbar\dot{a}\dfrac{k_{1n}^2 + k_{2n}^2}{k_{1n}k_{2n}}\dfrac{\partial k_{1n}}{\partial a}\left[\dfrac{1}{k_{2n}}\dfrac{\partial}{\partial r}r - \mathrm{i}a\dfrac{h_{l-1}}{h_l} + \dfrac{l}{k_{2n}}\right], & r > a(t) \end{cases}$$

视为

$$\hat{\mathscr{H}}_{r0} = \begin{cases} \hat{\mathrm{H}}_{r1} + q\varphi_1', & 0 \leqslant r \leqslant a(t); \\ \hat{\mathrm{H}}_{r2} + q\varphi_1', & r > a(t) \end{cases}$$

的微扰.将对应于 $\hat{\mathscr{H}}_{r0}$的能量本征值为 $\mathrm{E}_{l,n} + q\varphi_1'$ 取为零级近似 $\mathrm{E}_{l,n}'^{(0)}$,容易得到非厄米哈密顿算符 $\hat{\mathscr{H}}_r$ 的瞬时本征方程准确到一阶的解为(其他情况的本征态解我们将在别处讨论)

$$\mathrm{E}_{l,n}' = \mathrm{E}_{l,n}'^{(0)} + \mathrm{E}_{l,n}'^{(1)}; \quad |\mathscr{R}_n\rangle = |\mathscr{R}_n^{(0)}\rangle + |\mathscr{R}_n^{(1)}\rangle, \tag{58}$$

其中

$$\mathrm{E}_{l,n}'^{(0)} = \mathrm{E}_{l,n} + q\varphi_1', \tag{59}$$

$$|\mathscr{R}_n^{(0)}\rangle = |\chi_{r,n}^{(0)}\rangle = |\mathrm{R}_n\rangle, \tag{60}$$

$$\begin{aligned} \mathrm{E}_{l,n}'^{(1)} &= \langle \chi_{r,n}^{(0)} | \hat{\mathscr{H}}_r' | \mathscr{R}_n^{(0)} \rangle \\ &= \mathrm{i}\hbar\dot{a}\frac{k_{1n}^2 + k_{2n}^2}{k_{1n}k_{2n}}\frac{\partial k_{1n}}{\partial a}\mathrm{B}_{l,n}^2\left\{-\left[\frac{\mathrm{i}a^4}{2} + \frac{\mathrm{i}a^2(2l+1)^2}{8k_{2n}^2}\right]h_l h_{l-1}\right. \\ &\quad - \frac{\mathrm{i}a^4 h_{l-1}}{2h_l}\left(h_{l-1} - \frac{2l+1}{2\mathrm{i}k_{2n}a}h_l\right)^2 + \left[\frac{(2l+1)a^3}{4} + \frac{(2l-1)(2l+1)a}{16k_{2n}^2}\right]\frac{h_l^2}{k_{2n}} \\ &\quad \left. + \frac{(2l-1)a^3}{4k_{2n}}\left(h_{l-1} - \frac{2l+1}{2\mathrm{i}k_{2n}a}h_l\right)^2\right\}, \end{aligned} \tag{61}$$

令 $\hat{\mathscr{H}}_r'$中的$\dfrac{1}{\mathrm{i}k_{2n}}\dfrac{\partial}{\partial r}r - a\dfrac{h_{l-1}}{h_l} + \dfrac{l}{\mathrm{i}k_{2n}} = \hat{\mathscr{H}}_r''$,则

$$|\mathscr{R}_n^{(1)}\rangle = \hbar\dot{a}\frac{k_{1n}^2 + k_{2n}^2}{k_{1n}k_{2n}}\frac{\partial k_{1n}}{\partial a}\mathrm{B}_{l,n}\sum_{m\neq n}\frac{\mathrm{B}_{l,m}\langle h_l(\mathrm{i}k_{2m}r)|\hat{\mathscr{H}}_r''|h_l(\mathrm{i}k_{2n}r)\rangle}{\mathrm{E}_{l,n} - \mathrm{E}_{l,m}}|\mathrm{R}_m\rangle. \tag{62}$$

(62)式中

$$\begin{aligned} \langle h_l(\mathrm{i}k_{2m}r)|\hat{\mathscr{H}}_r''|h_l(\mathrm{i}k_{2n}r)\rangle &= \frac{\mathrm{i}k_{2m}a^3}{(k_{2n}^2 - k_{2m}^2)}\left(h_{l-1,k_n} - \frac{2l+1}{2\mathrm{i}k_{2n}a}h_{l,k_n}\right)\left(h_{l-1,k_m} - \frac{2l+1}{2\mathrm{i}k_{2m}a}h_{l,k_m}\right) \\ &\quad + \frac{4\mathrm{i}a^3k_{2n}^2 + \mathrm{i}a(2l+1)^2}{4k_{2n}(k_{2n}^2 - k_{2m}^2)}h_{l,k_n}h_{l,k_m} \end{aligned}$$

$$+\left[\frac{(2l-3)k_{2n}^2-(2l+1)k_{2m}^2}{2k_{2n}(k_{2n}^2-k_{2m}^2)^2}-\frac{\mathrm{i}ah_{l-1,k_n}}{(k_{2n}^2-k_{2m}^2)h_{l,k_m}}\right]$$

$$\times\left[k_{2m}a^2h_{l,k_n}\left(h_{l-1,k_m}-\frac{2l+1}{2\mathrm{i}k_{2m}a}h_{l,k_m}\right)-k_{2n}a^2h_{l,k_m}\left(h_{l-1,k_n}-\frac{2l+1}{2\mathrm{i}k_{2n}a}h_{l,k_n}\right)\right].\quad(63)$$

这里 $h_{l,k_n}=h_l(\mathrm{i}k_{2n}a)$. 由此得到 $\hat{H}'_r$ 瞬时能量本征态为

$$|R'_n\rangle=\hat{U}_2|\mathscr{R}_n\rangle=\hat{U}_2(|\mathscr{R}_n^{(0)}\rangle+|\mathscr{R}_n^{(1)}\rangle).\quad(64)$$

同理可求出 $\hat{H}_r'^{\dagger}$ 的瞬时能量本征方程的微扰展开到一阶的解为

$$E_{l,n}'^{*}=E_{l,n}-q\varphi_1'-E_{l,n}'^{(1)},\quad(65)$$

$$\langle\chi'_{r,n}|=\langle\chi_{r,n}|\hat{U}_2^{\dagger}=(\langle\chi_{r,n}^{(0)}|+\langle\chi_{r,n}^{(1)}|)\hat{U}_2^{\dagger}=(\langle\mathscr{R}_n^{(0)}|+\langle\mathscr{R}_n^{(1)}|)\hat{U}_2^{\dagger}.\quad(66)$$

当 $a(t)$做缓慢的周期变化时,系统经过一个周期 T 的时间演化后,由 $\hat{H}'_r$ 所确定的波函数的动力学相位为

$$-\frac{\mathrm{i}}{\hbar}\int_0^T(E_{l,n}+q\varphi_1'+E_{l,n}'^{(1)})\mathrm{d}t.\quad(67)$$

按公式(18),并利用(64)和(66)两式,且注意到$\langle R_m|R_n\rangle=\delta_{mn}$,可求得此波函数的复 Berry 相位为

$$\gamma_c=-\int_0^T\langle R_n|\left(\frac{\partial}{\partial t}f_2\right)|R_n\rangle\mathrm{d}t+2\mathrm{i}\int_0^T\langle R_n|\left(\frac{\partial}{\partial t}|\mathscr{R}_n^{(1)}\rangle\right)\mathrm{d}t$$
$$+\mathrm{i}\int_0^T\langle\chi_{r,n}^{(1)}|\hat{U}_2^{\dagger}\frac{\partial}{\partial t}(\hat{U}_2|\mathscr{R}_n^{(1)}\rangle)\mathrm{d}t,\quad(68)$$

其中

$$-\int_0^T\langle R_n|\left(\frac{\partial}{\partial t}f_2\right)|R_n\rangle\mathrm{d}t=-\int_0^T\langle R_n|r^2|R_n\rangle\left[\frac{m}{2\hbar k_{1n}}\frac{\partial k_{1n}}{\partial a}\mathrm{d}\dot{a}+\frac{m\dot{a}}{2\hbar}\mathrm{d}\left(\frac{1}{k_{1n}}\frac{\partial k_{1n}}{\partial a}\right)\right],\quad(69)$$

$$2\mathrm{i}\int_0^T\langle R_n|\left(\frac{\partial}{\partial t}|\mathscr{R}_n^{(1)}\rangle\right)\mathrm{d}t=2\mathrm{i}\hbar\int_0^T\frac{k_{1n}^2+k_{2n}^2}{k_{1n}k_{2n}}\frac{\partial k_{1n}}{\partial a}B_{l,n}$$
$$\times\sum_{m\neq n}\frac{B_{l,m}\langle h_l(\mathrm{i}k_{2m}r)|\hat{\mathscr{H}}_r''|h_l(\mathrm{i}k_{2n}r)\rangle}{E_{l,n}-E_{l,m}}\langle R_n|\left(\frac{\partial}{\partial t}|R_m\rangle\right)\mathrm{d}a,\quad(70)$$

$$\mathrm{i}\int_0^T\langle\chi_{r,n}^{(1)}|\hat{U}_2^{\dagger}\frac{\partial}{\partial t}(\hat{U}_2|\mathscr{R}_n^{(1)}\rangle)\mathrm{d}t\doteq\mathrm{i}\hbar^2\int_0^T\frac{(k_{1n}^2+k_{2n}^2)^2}{k_{1n}^2k_{2n}^2}\left(\frac{\partial k_{1n}}{\partial a}\right)^2B_{l,n}^2$$
$$\times\sum_{m\neq n}\frac{B_{l,m}^2(\langle h_l(\mathrm{i}k_{2m}r)|\hat{\mathscr{H}}_r''|h_l(\mathrm{i}k_{2n}r)\rangle)^2}{(E_{l,n}-E_{l,m})^2}\dot{a}\,\mathrm{d}\dot{a}.\quad(71)$$

上式中已忽略了 $\dot{a}(t)$的二次以上项. 而(69)式中的

$$\langle R_n|r^2|R_n\rangle=\frac{A_{l,n}^2a}{3}\left[\frac{a^4}{2}-\frac{(2l+1)^4-4(2l+1)^2}{(2k_{1n})^4}+\frac{(2l+1)^2a^2}{8k_{1n}^2}\right]j_l^2$$

$$- \frac{A_{l,n}^2 a}{3}\left[\frac{4a^2-(2l+1)^2a^2}{4k_{1n}^2}-\frac{a^4}{2}\right]\left[j_{l-1}-\frac{2l+1}{2k_{1n}a}j_l\right]^2$$
$$- \frac{A_{l,n}^2 a^4}{3k_{1n}}\left[j_{l-1}-\frac{2l+1}{2k_{1n}a}j_l\right]j_l+\left[\frac{(2l+1)^4-4(2l+1)^2}{(2k_{2n})^4}-\frac{a^4}{2}+\frac{(2l+1)^2a^2}{8k_{2n}^2}\right]$$
$$\times \frac{B_{l,n}^2 a}{3}h_l^2-\frac{B_{l,n}^2 a}{3}\left[\frac{a^4}{2}+\frac{4a^2-(2l+1)^2a^2}{4k_{2n}^2}\right]\left[h_{l-1}-\frac{2l+1}{2\mathrm{i}k_{2n}a}h_l\right]^2$$
$$+\frac{B_{l,n}^2 a^4}{3\mathrm{i}k_{2n}}\left[h_{l-1}-\frac{2l+1}{2\mathrm{i}k_{2n}a}h_l\right]h_l, \tag{72}$$

上式中 $j_l=j_l(k_{1n}a)$, $h_l=h_l(\mathrm{i}k_{2n}a)$. (70)式中的

$$\langle R_n|\frac{\partial}{\partial t}|R_m\rangle = A_{l,n}A_{l,m}\frac{\dot a\,\partial k_{1m}}{k_{1m}\partial a}\Bigg\{\frac{(2l+1)^2a-4k_{1m}^2a^3}{4(k_{1n}^2-k_{1m}^2)}j_{l,k_n}j_{l,k_m}$$
$$-\frac{k_{1n}k_{1m}a^3}{k_{1n}^2-k_{1m}^2}\left(j_{l-1,k_n}-\frac{2l+1}{2k_{1n}a}j_{l,k_n}\right)\left(j_{l-1,k_m}-\frac{2l+1}{2k_{1m}a}j_{l,k_m}\right)$$
$$+\frac{(k_{1n}^2-5k_{1m}^2)a^2}{2(k_{1n}^2-k_{1m}^2)^2}\Bigg[k_{1n}j_{l,k_m}\left(j_{l-1,k_n}-\frac{2l+1}{2k_{1n}a}j_{l,k_n}\right)-k_{1m}a^2j_{l,k_n}$$
$$\times\left(j_{l-1,k_m}-\frac{2l+1}{2k_{1m}a}j_{l,k_m}\right)\Bigg]\Bigg\}+A_{l,m}B_{l,n}\frac{\mathrm{i}a^2\dot a}{k_{2n}^2-k_{2m}^2}$$
$$\times\left[\left(k_{1m}+a\frac{\partial k_{1m}}{\partial a}\right)\frac{j'_{l,k_m}}{h_{l,k_m}}+\left(k_{2m}+a\frac{\partial k_{2m}}{\partial a}\right)\frac{j_{l,k_m}h'_{l,k_m}}{\mathrm{i}h_{l,k_m}^2}\right]$$
$$\times\left[k_{2m}h_{l,k_n}\left(h_{l-1,k_m}-\frac{2l+1}{2\mathrm{i}k_{2m}a}h_{l,k_m}\right)-k_{2n}h_{l,k_m}\left(h_{l-1,k_n}-\frac{2l+1}{2\mathrm{i}k_{2n}a}h_{l,k_n}\right)\right]$$
$$+B_{l,n}B_{l,m}\frac{\dot a\,\partial k_{2m}}{k_{2m}\partial a}\Bigg\{\frac{(2l+1)^2a+4k_{2m}^2a^3}{4(k_{2n}^2-k_{2m}^2)}h_{l,k_n}h_{l,k_m}$$
$$+\frac{k_{2n}k_{2m}a^3}{k_{2n}^2-k_{2m}^2}\left(h_{l-1,k_n}-\frac{2l+1}{2\mathrm{i}k_{2n}a}h_{l,k_n}\right)\left(h_{l-1,k_m}-\frac{2l+1}{2\mathrm{i}k_{2m}a}h_{l,k_m}\right)$$
$$+\frac{\mathrm{i}(5k_{2m}^2-k_{2n}^2)a^2}{2(k_{2n}^2-k_{2m}^2)}\Bigg[k_{2m}h_{l,k_n}\left(h_{l-1,k_m}-\frac{2l+1}{2\mathrm{i}k_{2m}a}h_{l,m}\right)$$
$$-k_{2n}h_{l,k_m}\left(h_{l-1,k_n}-\frac{2l+1}{2\mathrm{i}k_{2n}a}h_{l,k_n}\right)\Bigg]\Bigg\}, \tag{73}$$

上式中 $j_{l,k_m}=j_l(k_{1m}a)$, $h_{l,k_m}=h_l(\mathrm{i}k_{2m}a)$.

在 $V_0\to\infty$ 的极限情况下, $k_{2n}=\left[\frac{2m(V_0-E_{l,n})}{\hbar^2}\right]^{1/2}$ 也趋于∞. 因此有 $|R_{2n}\rangle=0$, $j_l(k_{1n}a)=0$. 令 $\beta_{n_r,l}$ 为 l 阶球贝塞尔函数的第 n_r 个根, 则 $k_{1n}=\frac{\beta_{n_r,l}}{a}$. 显然(70)和(71)两式为零. 由(45)式得

$$A_{l,n}=\left(\frac{a^3}{2}j_{l-1}^2\right)^{-1/2}, \tag{74}$$

按(72)式得

$$\langle R_n | r^2 | R_n \rangle = \left[\frac{1}{3} - \frac{4-(2l+1)^2}{6\beta^2_{n_r,l}}\right] a^2. \tag{75}$$

故此时的 Berry 相位变为

$$\begin{aligned}\gamma_c &= \frac{m}{2\hbar}\int_0^T \langle R_n | r^2 | R_n \rangle \left(\frac{\mathrm{d}\dot{a}}{a} - \frac{\dot{a}}{a^2}\mathrm{d}a\right) \\ &= \frac{m}{2\hbar}\left[\frac{1}{3} - \frac{4-(2l+1)^2}{6\beta^2_{n_r,l}}\right]\int_0^T (a\mathrm{d}\dot{a} - \dot{a}\,\mathrm{d}a).\end{aligned} \tag{76}$$

如果我们选取 $a(t) = a_0 + a_0'\sin\varphi(t)$, 且 $\alpha = \dot{\varphi} = \mathrm{const.}$, 则可得

$$\gamma_c = -\frac{m}{3\hbar}\left[1 - \frac{4-(2l+1)^2}{2\beta^2_{n_r,l}}\right] a_0'^2\,\alpha\pi. \tag{77}$$

这与文献[7]的结果一致,只是由于$\langle R_n | r^2 | R_n \rangle$的算法不一样,因而最后的形式不一样.

5 结语和讨论

本文用量子基础理论的方法分别从含时边界的一维半壁无限高势阱和含时边界的三维有限深球方势阱(角动量量子数 l 为偶数)构造了两个新哈密顿算符.它们对应于质量为 m 电荷为 q 的粒子在电磁场的作用下的新量子体系.值得指出的是,这两个新哈密顿量不再是厄米算符,从而描写开放和耗散系统.我们用微扰论的方法计算新量子体系波函数的复 Berry 相位,结果表明含时边界条件确实导致了 Berry 相因子.

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HAMILTONIAN OPERATORS CONSTRUCTED FROM TWO KINDS OF FINITE-DEPTH QUANTUM POTENTIAL WELLS WITH TIME-DEPENDENT BOUNDARY CONDITIONS AND THEIR COMPLEX BERRY PHASES *

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ABSTRACT

In the frame of the basic quantum theory, from the one-dimensional infinite-height half-wall quantum potential well with time-dependent boundary conditions and from the three-dimensional finite-depth sphere-square potential well with time-dependent boundary conditions we constructed two kinds of new Hamiltonian operators separately which describe electric particle interacting with eletromagnetic field. In the adiabatic approximation are calculated the complex Berry phases of two kinds of new systems.

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