

Preliminary Study on Ordering Problem in Potential Model

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Abstract While deriving the effective potential by calculating the elastic scattering amplitude between quark-antiquark, one would encounter the ordering problem. Even the hermiticity requirement is considered, various ordering schemes may still lead to different numerical results. We investigate this issue and present the preliminary results, then make some discussions.

Key words potential model, ordering scheme, quakonia, hermiticity

The non-relativistic potential model is proved to be a plausible approach to study spectra and wavefunctions of heavy quakonia^[1,2]. Except the mysterious confinement piece in the potential which should be input by hand, one can derive the leading-order pieces based on the perturbative QCD theory by calculating the elastic scattering amplitude of the constituent quarks.

When we write down the expressions of the scattering amplitude, all quantities are in the momentum space, so that they commute with each other. However, the Fourier transformation turns \mathbf{k} into its conjugate vector \mathbf{r} in the configuration space and leaves the momentum \mathbf{p} as a derivative operator, where \mathbf{k} is the exchanged 3-momentum between the quark and anti-quark, \mathbf{r} is the corresponding distance vector. Because \mathbf{p} and \mathbf{r} do not commute with each other, the ordering problem in the potential in the configuration space emerges and the problem is by no means trivial. Moreover, if we consider higher order terms of \mathbf{p}^2 in the non-relativistic reduction of the scattering amplitude, the ordering problem is even more serious.

In the earlier work^[3], the authors took a simple ordering scheme such as $f(r)\mathbf{p}^2$ and $f(r)\mathbf{r}\cdot(\mathbf{r}\cdot\mathbf{p})\mathbf{p}$ etc.. Evidently, these expressions are in general not Hermitian. Weyl noticed this problem^[4] and proposed the famous "Weyl ordering" scheme. Although this scheme is a convenient one to treat this problem, obviously it is not a unique choice and there is certain arbitrariness, so that we cannot allege that it is the best choice. Here "best" means that the solution obtained in the scheme is the closest one to the physical reality. Gromez presented an explicit expression when he discussed the effective Hamiltonian for heavy quarkonium^[5]. In his work, the spin-independent relativistic correction in the CM frame was written as

$$H_c = \frac{1}{4m^2} \nabla^2 V + \frac{1}{2m^2} \left\{ \left\{ \mathbf{p} \cdot V \mathbf{p} - \mathbf{p} \cdot \mathbf{r} \frac{V'}{r} \mathbf{r} \cdot \mathbf{p} \right\} \right\}_{\text{Weyl}}, \quad (1)$$

where $V' = \frac{dV}{dr}$ and the subscript "Weyl" denotes the Weyl ordering of the corresponding operators

Received 04 December 2001

* Supported by National Natural Science Foundation of China (19835060)

$$\{ | p_i V_{ij} p_j \} \}_{\text{weyl}} \equiv \frac{1}{4} [p_i p_j V_{ij} + 2 p_i V_{ij} p_j + V_{ij} p_i p_j] . \quad (2)$$

In Eq. (2), V_{ij} can be either $V\delta_{ij}$ or $V'r_i r_j / r$.

There is another commonly adopted ordering scheme so called as the Bohm ordering scheme^[6]. According to the scheme, the operator which corresponds to the classical quantity $f(x)g(p)$ is

$$\{ f(x)g(p) \}_{\text{Bohm}} = \frac{f(x)g(p) + g(p)f(x)}{2} . \quad (3)$$

Obviously, it is interesting to investigate whether there are other schemes and how different schemes influence the calculated results for the energy gap. To be explicit, we take the Cornell potential

$$V(r) = -\frac{\kappa}{r} + \sigma r, \kappa = \frac{4\alpha_s}{3} \quad (4)$$

for heavy quarkonia as an example to investigate several possible ordering schemes, and then compare the results in different schemes, finally we raise our proposal about ordering.

First, we discuss the terms such as $\mathbf{p} \cdot \mathbf{r} \frac{V'}{r} \mathbf{r} \cdot \mathbf{p}$ in Eq. (1). In general, there are 12 independent combinations as

$$\begin{aligned} a1 &= u(\mathbf{e} \cdot \mathbf{p})(\mathbf{e} \cdot \mathbf{p}), a2 = u(\mathbf{e} \cdot \mathbf{p})(\mathbf{p} \cdot \mathbf{e}), a3 = u(\mathbf{p} \cdot \mathbf{e})(\mathbf{e} \cdot \mathbf{p}), a4 = u(\mathbf{p} \cdot \mathbf{e})(\mathbf{p} \cdot \mathbf{e}), \\ a5 &= (\mathbf{e} \cdot \mathbf{p})u(\mathbf{e} \cdot \mathbf{p}), a6 = (\mathbf{e} \cdot \mathbf{p})u(\mathbf{p} \cdot \mathbf{e}), a7 = (\mathbf{p} \cdot \mathbf{e})u(\mathbf{e} \cdot \mathbf{p}), a8 = (\mathbf{p} \cdot \mathbf{e})u(\mathbf{p} \cdot \mathbf{e}), \\ a9 &= (\mathbf{e} \cdot \mathbf{p})(\mathbf{e} \cdot \mathbf{p})u, a10 = (\mathbf{e} \cdot \mathbf{p})(\mathbf{p} \cdot \mathbf{e})u, a11 = (\mathbf{p} \cdot \mathbf{e})(\mathbf{e} \cdot \mathbf{p})u, \\ a12 &= (\mathbf{p} \cdot \mathbf{e})(\mathbf{p} \cdot \mathbf{e})u, \end{aligned} \quad (5)$$

where $u = rV'$ and $\mathbf{e} = \mathbf{r}/r$ is the unit vector. Another set of 12 different combinations such as $u(\mathbf{e} \cdot (\mathbf{e} \cdot \mathbf{p})\mathbf{p})$ etc. can be expressed in terms of the operators in Eq. (5) with the commutative relation $[x_i, p_j] = i\delta_{ij}$.

Apparently, operators $a6$ and $a7$ are Hermitian, and the others are not. In order to form operators that have physical meaning, we must re-combine operators $a1, \dots, a12$ into Hermitian forms. We have seven simplest Hermitian combinations. Of course, based on these combinations, one can construct many other Hermitian forms, but these seven independent operators are fundamental ones. They are

$$\begin{aligned} b1 &= \frac{1}{2}(a1 + a12) = \frac{1}{2}[u(\mathbf{e} \cdot \mathbf{p})(\mathbf{e} \cdot \mathbf{p}) + (\mathbf{p} \cdot \mathbf{e})(\mathbf{p} \cdot \mathbf{e})u], \\ b2 &= \frac{1}{2}(a2 + a10) = \frac{1}{2}[u(\mathbf{e} \cdot \mathbf{p})(\mathbf{p} \cdot \mathbf{e}) + (\mathbf{e} \cdot \mathbf{p})(\mathbf{p} \cdot \mathbf{e})u], \\ b3 &= \frac{1}{2}(a3 + a11) = \frac{1}{2}[u(\mathbf{p} \cdot \mathbf{e})(\mathbf{e} \cdot \mathbf{p}) + (\mathbf{p} \cdot \mathbf{e})(\mathbf{e} \cdot \mathbf{p})u], \\ b4 &= \frac{1}{2}(a4 + a9) = \frac{1}{2}[u(\mathbf{p} \cdot \mathbf{e})(\mathbf{p} \cdot \mathbf{e}) + (\mathbf{e} \cdot \mathbf{p})(\mathbf{e} \cdot \mathbf{p})u], \\ b5 &= \frac{1}{2}(a5 + a8) = \frac{1}{2}[(\mathbf{e} \cdot \mathbf{p})u(\mathbf{e} \cdot \mathbf{p}) + (\mathbf{p} \cdot \mathbf{e})u(\mathbf{p} \cdot \mathbf{e})], \\ b6 &= a6 = (\mathbf{e} \cdot \mathbf{p})u(\mathbf{p} \cdot \mathbf{e}), \\ b7 &= a7 = (\mathbf{p} \cdot \mathbf{e})u(\mathbf{e} \cdot \mathbf{p}). \end{aligned} \quad (6)$$

Here we would set the hermiticity to be the first criterion for any ordering scheme. Below we will discuss some other criteria which may only apply to specific potential forms.

We first consider the Coulomb part of the Cornell potential Eq. (4), because it brings up a singularity problem which needs to be dealt with carefully. Taking $V = -1/r$, then $u = rV' = 1/r$,

$\nabla^2 V = -\nabla^2 \frac{1}{r} = 4\pi\delta(\mathbf{r})$. Consequently,

$$\begin{aligned} b1 &= -2\pi\delta^3(\mathbf{r}) + \tilde{b}, & b2 &= \frac{2}{r^3} + 2\pi\delta(\mathbf{r}) + \tilde{b}, \\ b3 &= 2\pi\delta(\mathbf{r}) + \tilde{b}, & b4 &= -\frac{2}{r^3} + 2\pi\delta(\mathbf{r}) + \tilde{b}, \\ b5 &= -4\pi\delta(\mathbf{r}) + \tilde{b}, & b6 &= \frac{4}{r^3} + \tilde{b}, \\ b7 &= \tilde{b}, \end{aligned}$$

where

$$\tilde{b} = -\frac{1}{r^2} \frac{\partial}{\partial r} - \frac{1}{r} \frac{\partial^2}{\partial r^2}. \quad (8)$$

As pointed out by Landau, if a potential is more singular than $1/r^2$, the Schrödinger equation is unsolvable.^{7,8)} In the expressions of b s, two kinds of terms are more singular than $1/r^2$. They involve $\delta^3(\mathbf{r})$ and $1/r^3$, respectively. The first one in general is sufficiently benign in the perturbative calculation. It provides a correction which can be calculated by using the wave function at origin. However, the second one that shows up in $b2$, $b4$ and $b6$ is intolerable, because it results in non-physical divergence in the S -states. A simple hermitizing procedure proposed in Eq. (6) cannot eliminate these troublesome divergent terms. Indeed, the other forms of effective potentials which are commonly used for the quarkonia, such as the linear potential or the logarithm potential etc., would not produce terms which are more singular than $1/r^2$ at $r \rightarrow 0$ and do not cause principal difficulties in calculations. For these potentials, the hermiticity requirement would be enough as a criterion of ordering scheme. However, when we choose the Cornell potential as the zero-th order perturbative potential to calculate the spectra of quarkonia, some ordering schemes would produce divergent terms such as $1/r^3$. To avoid contradiction with real physics, this kind of terms should reasonably be evaded by selecting proper ordering schemes.

It is easy to see that besides the trivial terms $b1$, $b3$, $b7$, the simplest non-divergent combinations can be

$$\frac{1}{2}(b2 + b4) = 2\pi\delta(\mathbf{r}) + \tilde{b} = b3$$

and

$$\frac{1}{3}(2b4 + b6) = \frac{4}{3}\pi\delta(\mathbf{r}) + \tilde{b} = \frac{2}{3}b3 + \frac{1}{3}\tilde{b}.$$

It is interesting to re-write the result of the Weyl ordering

$$\{p_i V_{ij} p_j\}_{\text{Weyl}} = -\pi\delta(\mathbf{r}) + \tilde{b}, \quad (9)$$

which is Hermitian and free of the singularity $1/r^3$.

To show the results from different ordering schemes, we calculate the energy gap between the $2S$ and $1S$ states of the cc system. The resultant first order relativistic corrections from spin-independent term $-\frac{1}{2m^2}\mathbf{p} \cdot \mathbf{r} \frac{V'}{r} \mathbf{r} \cdot \mathbf{p}$ in various ordering schemes are tabulated in Table 1.

We also investigate the simpler term $\mathbf{p} \cdot V\mathbf{p}$. Its expression in the Weyl ordering scheme is $\frac{(\mathbf{p}^2 V + 2\mathbf{p} \cdot V\mathbf{p} + V\mathbf{p}^2)}{4}$ and in the Bohm ordering scheme reads $\frac{(\mathbf{p}^2 V + V\mathbf{p}^2)}{2}$. For the Coulomb potential, the ordering scheme can be expressed in a generalized form

$$(1-a)\left(\frac{(\mathbf{p}^2 V + V\mathbf{p}^2)}{2}\right) + a\mathbf{p} \cdot V\mathbf{p} = -(1-a)b3 - a\tilde{b},$$

where a is a free parameter. The Weyl ordering corresponds to $a = 0.5$, namely

$$\frac{(p^2 V + V p^2 + 2p \cdot V p)}{4} = -\frac{(b3 + \tilde{b})}{4},$$

and the Bohm ordering scheme requires $a = 0$. For various values of the parameter a , the numerical results would deviate about 5—15 MeV for $0 \leq a \leq 1$ for J/ψ .

Table 1. The corrections from the first order perturbation term $-\frac{1}{2m^2} p \cdot r \frac{V'}{r} r \cdot p$ for the energy gap between the 2S and 1S states of the $c \bar{c}$ system in different ordering schemes.

Ordering scheme	c. v. from Coulomb part/MeV	c. v. from Linear part/MeV	Total c. v./MeV
$b1$	- 26.6	- 44.0	- 70.6
$b3$	- 13.8	- 25.4	- 39.2
$b5$	- 46.9	- 34.7	- 81.6
$b7$	- 6.3	- 16.1	- 22.4
$\frac{1}{2}(b2 + b4)$	34.3	- 16.1	18.2
$\frac{1}{3}(2b2 + b6)$	7.2	- 19.3	- 12.1
$(e \cdot p) u (e \cdot p)_{\text{Bohm}} = b1$	- 26.6	- 44.0	- 70.6
$(e \cdot p) u (e \cdot p)_{\text{Weyl}} = \frac{b1 + b7}{2}$	- 16.5	- 30.1	- 46.6

The zero-th order potential is the Cornell potential $V(r) = \frac{-4\alpha_s}{3r} + \sigma r$ with $m_c = 1.84\text{GeV}$, $\alpha_s = 0.39$, $\sigma = 0.182\text{GeV}^2$. The energy gap in the zero-th order approximation is $E_{2S} - E_{1S} = 592.7\text{MeV}$. c. v. denotes the value of the first order correction.

We have achieved the following observations:

(1) In selecting ordering scheme, the operators in the scheme should be Hermitian, otherwise some absurd values would appear and produce non-physical results.

(2) One can expect numerical deviations from one ordering scheme to the others, the range is about several tens of MeV.

(3) The resultant corrections and the degrees of deviations in different ordering schemes depend on the potential forms in the zero-th order approximation.

In fact, the ordering phenomenon also exists in the variational calculator where the potential includes aforementioned relativistic correction terms. It is found, in our previous work, that the ordering effect is usually absorbed into the values of variational parameters via the variational operation. Namely, in different ordering schemes, the values of variational parameters are different, but the resultant physical quantities are very close^[9].

As the conclusion of this work, we find:

1. Choosing a proper ordering scheme, which originates from the Fourier transformation in deriving a non-relativistic potential from the quantum field theory, is important, non-negligible and unavoidable in the investigation of hadronic physics.

2. In the non-relativistic potential model, calculated results depend on the form of the employed potential, the values of model parameters, and the scheme of ordering the operators.

3. A proper ordering scheme should at least satisfy two conditions: the potential operators should be Hermitian, and should not cause the divergent disaster.

4. Phenomenological model is still a basis to study hadronic physics, because it is simple and can grasp the major essence. For a specific potential model and model parameters, if the aforementioned two conditions are satisfied, the scheme is possible to be a proper one to fit the data. Then, in the further study of new physics, the results would be self consistent and meaningful. We notice that

both the Weyl and Bohm's schemes possess the required properties, so can be applied in the practical calculations, a difference in numbers can be expected, but it is no more than a few tens of MeV. This difference might bring up some phenomenological consequence along with the effects of other corrections such as the loop effects and higher order relativistic corrections, as the measurement becomes more and more precise. So the choice of the ordering scheme indeed stands as a serious problem in the potential model and is worth more attention of theorists.

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势模型中排序问题的初步研究*

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摘要 由动量空间计算得到的夸克和反夸克之间的散射振幅推导坐标空间等效势时, 总要出现算符排序问题, 这是一个量子力学中长期存在而又未能得到很好解决的重要问题. 以重夸克偶素中常用的 Cornell 势为例, 重新进行了研究, 给出了一些初步的结果. 指出即使考虑了厄米性的要求, 各种排序方案仍然会导致有很大差别的数值结果, 会严重影响谱的拟合精度. 对这些结果的意义及其相关问题作了一些讨论.

关键词 势模型 排序方案 夸克偶素 厄米性

2001-12-04 收稿

* 国家自然科学基金(19835060)资助