Вычисление логарифма Бете

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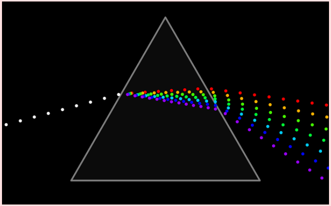


ФФК-11, декабрь 2011

Motivation

Transition lines in HD^+:

	$(L,v)=(0,0)\to(0,1)$	$(L,v)=(0,0)\to(1,0)$
ΔE_{nr}	57 349 439.9717	1 314 886.777 28
ΔE_{α^2}	958.152(03)	48.4161(06)
ΔE_{α^3}	−242.125(02)	−9.3789(16)
ΔE_{α^4}	−1.748	−0.0682
ΔE_{α^5}	0.105(19)	0.0040(08)
ΔE_{tot}	57 350 154.355(21)	1 314 925.7510(22)

The $\alpha(Z\alpha)^2 E_{nr}$ order low-energy contribution may be written

$$E_{L0} = \frac{\alpha^3}{4\pi^2} \int_{|\mathbf{k}|<\Lambda} \frac{d^3k}{k} \left(\delta^{ij} - \frac{k^i k^j}{k^2}\right) \left\langle \psi_0 \middle| p^i \left(\frac{1}{E_0 - H - k}\right) p^j \middle| \psi_0 \right\rangle - \delta m \langle \psi_0 | \psi_0 \rangle$$

Averaging over angular variables one gets

$$E_{L0} = \frac{2\alpha^3}{3\pi} \int_0^\Lambda k\, dk \left\langle \mathbf{p} \left(\frac{1}{E_0 - H - k}\right) \mathbf{p} \right\rangle - \delta m \langle \psi_0 | \psi_0 \rangle$$

Radiative correction. Low energy contribution

The asymptotic behaviour of the integrand for large k can be expressed using the following expansion

$$(E_0-H-k)^{-1} = -1/k - \frac{1}{k^2}(E_0-H) + \frac{1}{k^2}\frac{(E_0-H)^2}{E_0-H-k}$$

that results in

$$E_{L0} = \frac{2\alpha^3}{3\pi}\left[-\left\langle \mathbf{p}^2\right\rangle \Lambda + \langle \mathbf{p}\,[H,\mathbf{p}]\rangle \ln\Lambda + \int \frac{dk}{k}\left\langle \mathbf{p}\frac{(E_0-H)^2}{E_0-H-k}\mathbf{p}\right\rangle\right] - \delta m$$

As was shown by Bethe in 1948, the linearly divergent term may be associated with "mass renormalization" of an electron.

Radiative correction. Low energy contribution

The nonlogarithmic contribution may now be defined as

$$E_{L0} = \frac{2\alpha^3}{3\pi}\int_0^{E_h} k\,dk \left\langle \mathbf{p}\left(\frac{1}{E_0-H-k}+\frac{1}{k}\right)\mathbf{p}\right\rangle + \frac{2\alpha^3}{3\pi}\int_{E_h}^{\infty}\frac{dk}{k}\left\langle \mathbf{p}\frac{(E_0-H)^2}{E_0-H-k}\mathbf{p}\right\rangle$$

here E_h is the Hartree energy. The contribution from

$$\frac{2\alpha^3}{3\pi}\left(\int_{E_h}^{\Lambda}\frac{dk}{k}\right)\left\langle \mathbf{p}\,[H,\mathbf{p}]\right\rangle = \frac{2\alpha^3}{3\pi}\ln\frac{\Lambda}{E_h}\;\left(4\pi Z\langle\delta(\mathbf{r})\rangle\right)$$

results in appearance of the logarithmic term, the cut-of parameter is later canceled out by the logarithmic term from the high energy part. The formal expression for the Bethe logarithm may be written as follows:

$$\beta(nl) = \frac{\sum_{n\neq 0}\langle 0|\,p\,|n\rangle^2 (E_n-E_0)\ln(|E_n-E_0|/E_h)}{\sum_{n\neq 0}\langle 0|\,p\,|n\rangle^2 (E_n-E_0)}$$

Radiative correction. High energy contribution

The high energy contribution is obtained from the one-loop scattering amplitude for an electron in an external field

$$M_1 = \frac{\alpha}{2\pi}\left[2\left(\ln\frac{m}{\lambda_{min}}-1\right)\left(1-\frac{2\theta}{\tan 2\theta}\right)+\theta\tan\theta + \frac{4}{\tan 2\theta}\int_0^\theta \alpha\tan\alpha\, d\alpha\right]a_\nu\gamma^\nu + \frac{\alpha}{2\pi}\left[\frac{i}{2m}q_\mu a_\nu \Sigma^{\mu\nu}\frac{2\theta}{\sin 2\theta}+r\, a_\nu\gamma^\nu\right],$$

where

$$\Sigma^{\mu\nu} = (\gamma^\mu\gamma^\nu-\gamma^\nu\gamma^\mu)/(2i), \qquad r = \ln(\lambda/m)+9/4-2\ln(m/\lambda_{min}),$$

$$q^2 = 4m^2\sin^2\theta.$$

Radiative correction. High energy contribution

At small q, scattering amplitude may be rewritten:

$$M_1 \approx \frac{\alpha}{\pi}\left[\left(-\frac{1}{8m^2}+\frac{1}{3m^2}\ln\frac{m}{\lambda_{min}}\right)a_\nu\gamma^\nu q^2+\frac{i}{4m}q_\mu a_\nu\Sigma^{\mu\nu}\right]$$
$$+\frac{\alpha}{\pi}\left[\left(-\frac{11}{240m^4}+\frac{1}{20m^4}\ln\frac{m}{\lambda_{min}}\right)a_\nu\gamma^\nu q^4+\frac{i}{24m^3}q_\mu a_\nu\Sigma^{\mu\nu}q^2\right]$$

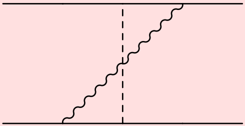
The leading order contribution for a *static scalar field* with "renormalization" to a new infrared regularization parameter Λ, which is a cut-off of virtual quanta of momentum less than Λ:

$$M_1^{(0)} = -\frac{\alpha}{3\pi}\frac{\mathbf{q}^2}{m^2}\left(\ln\frac{m}{2\Lambda}+\frac{5}{6}-\frac{3}{8}\right)a_0+\frac{\alpha}{2\pi}\frac{1}{m^2}\left(-\frac{\mathbf{q}^2}{4}+\frac{i\boldsymbol{\sigma}[\mathbf{q}\times\mathbf{p}]}{2}\right)a_0$$

In order to get this expression $\ln m/\lambda_{min}$ should be replaced by $(\ln m/\Lambda+5/6)$[1].

[1]R.P. Feynman, Phys. Rev. **76**, 769 (1949), footnote 13

The $\alpha(Z\alpha)^2(m/M)E_{nr}$ order low-energy contribution may be written



$$E_{L0}^{ret}(a,b) = \frac{\alpha^3}{(4\pi)^2}\int_{|\mathbf{k}|<\Lambda}\frac{d\mathbf{k}}{k}\left(\delta^{ij}-\frac{k^i k^j}{k^2}\right)\left\langle\phi\left|\frac{p_a^i}{m_a}\left(\frac{1}{E_0-k-H_0}+\frac{1}{k}\right)\frac{p_b^j}{m_b}\right|\phi\right\rangle$$

The total contribution for the many particle system may be expressed in terms of an electric current density operator

$$\mathbf{J} = \sum_i \frac{z_i}{m_i}\mathbf{P}_i,$$

Bethe logarithm

The Bethe log may be then defined as follows:

Numerator:

$$\mathcal{N}(L,v) = \int_0^{E_h} k\,dk \left\langle \mathbf{J} \left(\frac{1}{E_0-H-k} + \frac{1}{k} \right) \mathbf{J} \right\rangle + \int_{E_h}^{\infty} \frac{dk}{k} \left\langle \mathbf{J} \frac{(E_0-H)^2}{E_0-H-k} \mathbf{J} \right\rangle$$

Denominator:

$$\mathcal{D}(L,v) = \left\langle \mathbf{J}\,[H,\mathbf{J}] \right\rangle$$

and then the Bethe log itself as a ratio

$$\beta(L,v) = \frac{\mathcal{N}}{\mathcal{D}}\,.$$

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and then the Bethe log itself as a ratio

$$\beta(L,v) = \frac{\mathcal{N}}{\mathcal{D}}\,.$$

First order perturbation WF: $\psi_1(\cdot)$

A general procedure is to calculate

$$J(k) = \left\langle \mathbf{J}\,(E_0 - H - k)^{-1}\,\mathbf{J} \right\rangle$$

by solving equation

$$(E_0 - H - k)\psi_1 = i\mathbf{J}\psi_0,$$

for different values of k. As a first approximation one may take

$$\psi_1^{(0)} = -(i/k)\mathbf{J}\psi_0.$$

First order perturbation WF: $\psi_1(\cdot)$

Any approximate solution for ψ_1 may be iteratively improved:

$$\psi_1^{(n)} = -\frac{i}{k}\mathbf{J}\psi_0 + \frac{1}{k}(E_0 - H)\psi_1^{(n-1)}$$

and

$$\psi_1^{(1)} = -\frac{i}{k}\mathbf{J}\psi_0 + \frac{1}{k^2}\left[H, i\mathbf{J}\right]\psi_0$$

where

$$[H, i\mathbf{J}] = \sum_{i>j} z_i z_j \left(\frac{z_j}{m_j} - \frac{z_i}{m_i}\right)\frac{\mathbf{r}_{ij}}{r_{ij}^3}\,, \qquad \mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i.$$

First order perturbation WF: $\psi_1(\cdot)$

At small r_{ij}, ψ_1 is smooth and is described by an approximate equation

$$\left(\frac{1}{2m_{ij}}\Delta_{ij} - k\right)\psi_1(r_{ij},\cdot) = 0$$

that gives homogeneous solutions of the type

$$\sim \frac{\mathbf{r}_{ij}}{r_{ij}^3}\, e^{-\mu_{ij} r_{ij}}\,(1 + \mu_{ij} r_{ij})$$

with $\mu_{ij} = \sqrt{2m_{ij}k}$.

$$\psi_1^{(1)} = -\frac{i}{k}\mathbf{J}\psi_0(\cdot) + \frac{1}{k^2}\,[H, i\mathbf{J}]\left[1 - \sum_{i>j} e^{-\mu_{ij} r_{ij}}\,(1 + \mu_{ij} r_{ij})\right]\psi_0(\cdot)\,.$$

Asymptotic of $J(k)$ at $k \to \infty$.

Integrand

$$J(k) = \left\langle \mathbf{J}\,(E_0 - H - k)^{-1}\,\mathbf{J} \right\rangle$$

may be evaluated using the variational formalism as a stationary solution of a functional on ψ_1

$$J(k) = -2\,\langle\psi_0|i\mathbf{J}|\psi_1\rangle - \langle\psi_1(E_0 - H - k)\psi_1\rangle$$

To get asymptotic expansion we substitute $\psi_1^{(1)}$ into this functional.

Asymptotic of $J(k)$: $r_{ij} \longrightarrow 0$

At small r_{ij} one gets

$$
\begin{aligned}
J_{\rho_-} &= -\left\langle \psi_1^{(1)}(E_0 - H - k)\psi_1^{(1)} \right\rangle_{\rho_-} \\
&= -\frac{1}{k^3}\sum_{i>j} z_i^2 z_j^2 \left(\frac{z_i}{m_i} - \frac{z_j}{m_j}\right)^2 \left[\sqrt{2m_{ij}k} + \right. \\
&\qquad \left. + z_i z_j m_{ij}\Big(\ln(m_{ij}k) - \ln 2 + 1 + 2\gamma_E + 2\ln\rho\Big)\right] 4\pi\,\langle\delta(\mathbf{r}_{ij})\rangle
\end{aligned}
$$

where ρ_- means integration from 0 to ρ.

Asymptotic of $J(k)$: regular r_{ij}

For regular r_{ij} we use $\psi_1^{(1)}$ in a form:

$$\psi_1^{(1)} = -\frac{i}{k}\mathbf{J}\psi_0 + \frac{1}{k^2}\left[H, i\mathbf{J}\right]\psi_0$$

Then

$$-2\left\langle \psi_0 | i\mathbf{J} | \psi_1^{(1)} \right\rangle = -\frac{2}{k}\left\langle \mathbf{J}^2 \right\rangle - \frac{2}{k^2}\,\frac{\langle\, [i\mathbf{J}, [H, i\mathbf{J}]]\,\rangle}{2}$$

and

$$-\left\langle \psi_1^{(1)}(E_0 - H - k)\psi_1^{(1)} \right\rangle_{\rho_+} = k\left\langle \psi_1^{(1)} \middle| \psi_1^{(1)} \right\rangle_{\rho_+} - \left\langle \psi_1^{(1)}(E_0 - H)\psi_1^{(1)} \right\rangle_{\rho_+}$$

$$= \frac{1}{k}\left\langle \mathbf{J}^2 \right\rangle + \frac{1}{k^2}\,\frac{\langle\, [i\mathbf{J}, [H, i\mathbf{J}]]\,\rangle}{2}$$

$$-\frac{1}{k^3}\left[\left\langle\, [H, i\mathbf{J}]^2\,\right\rangle_{\rho_+} - \sum_{i>j} \frac{z_i^2 z_j^2\, m_{ij}}{\rho_{ij}}\, 4\pi \left\langle \delta(\mathbf{r}_{ij}) \right\rangle \right]$$

Asymptotic of $J(k)$: Hydrogen ground state

Hamiltonian

$$H = -\frac{\boldsymbol{\nabla}^2}{2} - \frac{Z}{r}, \qquad i\mathbf{J} = -\boldsymbol{\nabla}.$$

Commutations

$$[H, \boldsymbol{\nabla}] = -Z\frac{\mathbf{r}}{r^3},$$

$$[\boldsymbol{\nabla}, [H, \boldsymbol{\nabla}]] = -4\pi Z \langle\delta(\mathbf{r})\rangle .$$

Variational functional

$$J(k) = -2\langle\psi_0|\boldsymbol{\nabla}|\psi_1\rangle - \langle\psi_1(E_0 - H - k)\psi_1\rangle$$

Asymptotic of $J(k)$: Hydrogen ground state

- For $r<\rho$ ($\rho\to 0$, and $\mu\rho\gg 0$):

$$J_{\rho_-} = 4\pi\left\langle\delta(\mathbf{r})\right\rangle Z^{-3}\left[-\frac{Z^5\sqrt{2k}}{k^3}+\frac{Z^6(\ln k-\ln 2+1)}{k^3}+\frac{2Z^6(\gamma_E+\ln\rho)}{k^3}\right]$$

- For $r>\rho$:

$$\begin{aligned}J_{\rho_+} &= \frac{1}{k}\left\langle\boldsymbol{\nabla}^2\right\rangle-\frac{1}{k^2}\frac{\left\langle\,[\boldsymbol{\nabla},[H,\boldsymbol{\nabla}]]\,\right\rangle}{2}-\frac{1}{k^3}\left[\left\langle\,[H,\boldsymbol{\nabla}]^2\,\right\rangle_{\rho+}-\frac{Z^2}{\rho}4\pi\left\langle\delta(\mathbf{r})\right\rangle\right]\\ &= -\frac{Z^2}{k}+\frac{2Z^4}{k^2}-\frac{8Z^6\left[\gamma_E+\ln(2Z\rho)\right]}{k^3}+\dots\end{aligned}$$

Summing up

$$\begin{aligned}J(k) &= \frac{1}{k}\left\langle\boldsymbol{\nabla}^2\right\rangle-\frac{1}{k^2}\frac{\left\langle\,[\boldsymbol{\nabla},[H,\boldsymbol{\nabla}]]\,\right\rangle}{2}-\frac{1}{k^3}\left[\left\langle\,[H,\boldsymbol{\nabla}]^2\,\right\rangle_{\rho+}-\frac{Z^2}{\rho}4\pi\left\langle\delta(\mathbf{r})\right\rangle\right]\\ &\quad+\left[-\frac{Z^5\sqrt{2k}}{k^3}+\frac{Z^6(\ln k-\ln 2+1)}{k^3}+\frac{2Z^6(\gamma_E+\ln\rho)}{k^3}\right]Z^{-3}4\pi\left\langle\delta(\mathbf{r})\right\rangle\\ &= -\frac{Z^2}{k}+\frac{2Z^4}{k^2}-\frac{4Z^5\sqrt{2k}}{k^3}+\frac{4Z^6(\ln k-\ln Z^2)}{k^3}-\frac{4Z^6(3\ln 2-1)}{k^3}+\dots\end{aligned}$$

Variational property

We consider a quantity

$$\mathcal{J}_\Lambda = \int_0^\Lambda k\,dk\,J(k) = \sum_n \left|\langle\psi_0|\mathbf{J}|\psi_n\rangle\right|^2 \left[\Lambda - (E_0 - E_n)\ln\left|\frac{E_0 - E_n}{E_0 - E_n - \Lambda}\right|\right].$$

For the ground states this quantity possesses the variational property, since for the integrand for all k the following inequality is fulfilled

$$J_{\text{exact}}(k) \geq J_{\text{numerical}}(k).$$

The same property remains satisfied for other states if integration is performed from some $k_0 \sim 1$, which lies above the poles related to the states $E_n < E_0$. It is known from the practical calculations that the low k contribution become numerically converged to a high accuracy at a moderate basis length of intermediate states, and thus with a good confidence the variational property, the higher the value of $\mathcal{J}_\Lambda$ the more accurate solution, is valid.

Basis set

- Regular basis set, as for initial state
- Special basis set with exponentially growing exponents for a particular r_{ij}

$$\begin{cases} A_1^{(0)} = A_1, & A_2^{(0)} = A_2 \\ A_1^{(n)} = \tau^n A_1, & A_2^{(n)} = \tau^n A_2 \end{cases}$$

  where $\tau = A_2/A_1$.
  Typically $[A_1, A_2] = [2.5, 4.5]$, and $n_{\max} = 5-7$, that corresponds to the photon energy interval $k \in [0, 10^4]$.
- Similar basis sets for other pairs of (i, j).

Numerical scheme

- We diagonalize matrix of the Hamiltonian H_I for intermediate states (to get a set of E_m), and calculate $\langle 0|i\mathbf{J}|m\rangle$.
- One may easily restore $J(k)$ from these data and integrate

$$\int_0^{E_h} k\,dk \left\langle \mathbf{J}\left(\frac{1}{E_0-H-k}+\frac{1}{k}\right)\mathbf{J}\right\rangle + \int_{E_h}^{\Lambda}\frac{dk}{k}\left\langle \mathbf{J}\frac{(E_0-H)^2}{E_0-H-k}\mathbf{J}\right\rangle$$

  the low energy part of the numerator $\mathcal{N}(L,v)$.
- From $J(k)$ we extrapolate coefficients of asymptotic expansion and get

$$\int_{\Lambda}^{\infty}\frac{dk}{k}\left\langle \mathbf{J}\frac{(E_0-H)^2}{E_0-H-k}\mathbf{J}\right\rangle, \qquad f_{\rm fit}(k)=\sum_{m=1}^{M}\frac{C_{1m}\sqrt{k}+C_{2m}\ln k+C_{3m}}{k^{m+3}}$$

  the high energy part of the numerator.
- The work is done!

Results

Hydrogen ground state


```
Parameters of perturbation states:
----------------------------------

    Orbital angular momentum l = 1

  Basis of the first type:
  ------------------------

    Number of parameter sets    n = 1
       [A_1, A_2]
    0.35000   0.80000       n(1) = 12

  Basis of the second type:
  -------------------------

    Number of parameter sets    n = 7
       [A_1, A_2]
    0.40000   1.20000       n(1) =  8
    1.20000   3.60000       n(2) =  8
    3.60000  10.80000       n(3) =  8
   10.80000  32.40000       n(4) =  8
   32.40000  97.20000       n(5) =  8
   97.20000 291.60000       n(6) =  8
  291.60000 874.80000       n(7) =  8

    The total number of basis functions =   68

    The upper limit of the integration =  100000.



 Extrapolation contribution from the interval [xmax,infty] = -0.234258E-06


 Bethe logarithm ln(k_0) =  2.984128555765498


 CPU time:    0 h  0 min  0.55 sec
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Ground state of helium

$N_b \setminus N_a$	3000	3500	4000	∞
4000	4.37016022311	4.37016022301	4.370160223021	
5000	4.37016022314	4.37016022303	4.370160223044	
6000		4.37016022304	4.370160223058	
∞				4.37016022306(2)

Ground state of hydrogen molecular ion H_2^+

$N_b \setminus N_a$	3000	4000	5000	∞
7000	3.0122303407	3.0122303334		
8000	3.0122303431	3.0122303357	3.0122303341	
9000	3.0122303442	3.0122303367	3.0122303349	
∞				3.012230335(1)