# On Fromm-Hill integral

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# Outline

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- Remiddi-Pachucki-Puchalski method
- The closed form derived by Fromm and Hill
- The future work

# Motivation

For few-body systems,

$$H = H_0 + H_{rel} + H_{QED} + \cdots$$

with $H_0$ a non-relativistic Hamiltonian and some corrections.

From Rayleigh-Ritz variational principle, we have a generalized eigenvalue problem

$$\underline{H_0}\,\underline{c} = \lambda \underline{O}\,\underline{c},$$
$$H_{0ij} = \langle \psi_i | H_0 | \psi_j \rangle,$$
$$O_{ij} = \langle \psi_i | \psi_j \rangle,$$

ie, we solve the eigenvalue problem for $H_0$ first.

Hylleraas-type wave functions are always chosen to be trial basis.

The basic integral

$$
\begin{aligned}
&J(n_1, n_2, n_3, n_{12}, n_{23}, n_{31}; \alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31}) \\
&= \int r_1^{n_1-1} r_2^{n_2-1} r_3^{n_3-1} r_{12}^{n_{12}-1} r_{23}^{n_{23}-1} r_{31}^{n_{31}-1} \\
&\times \exp(-\alpha_1 r_1 - \alpha_2 r_2 - \alpha_3 r_3 - \alpha_{12} r_{12} - \alpha_{23} r_{23} - \alpha_{31} r_{31}) \\
&\times d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3.
\end{aligned} \tag{1}
$$

The generating integral

$$
\begin{aligned}
&I(\alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31}) \\
&= \int \frac{\exp(-\alpha_1 r_1 - \alpha_2 r_2 - \alpha_3 r_3 - \alpha_{12} r_{12} - \alpha_{23} r_{23} - \alpha_{31} r_{31})}{r_1 r_2 r_3 r_{12} r_{23} r_{31}} \\
&\times d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3.
\end{aligned} \tag{2}
$$

"Generating" means that (1) can be derived from (2) by differentiation:

$$J(n_1, n_2, n_3, n_{12}, n_{23}, n_{31}; \alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31})$$
$$= \left(-\frac{\partial}{\partial \alpha_1}\right)^{n_1} \left(-\frac{\partial}{\partial \alpha_2}\right)^{n_2} \left(-\frac{\partial}{\partial \alpha_3}\right)^{n_3} \left(-\frac{\partial}{\partial \alpha_{12}}\right)^{n_{12}} \tag{3}$$
$$\times \left(-\frac{\partial}{\partial \alpha_{23}}\right)^{n_{23}} \left(-\frac{\partial}{\partial \alpha_{31}}\right)^{n_{31}} I(\alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31})$$

- Nonrelativistic case: the integers $n_1$, $n_2$, $n_3$, $n_{12}$, $n_{23}$ and $n_{31}$ are all nonnegative.
- Leading relativistic corrections: some of the integers are equal to -1.
- QED corrections, etc.

# Remiddi-Pachucki-Puchalski method

Setting $\alpha_{\mu\nu} = 0$, the basic integral (1) is simplified to

$$\begin{aligned} &\tilde{J}(n_1, n_2, n_3, n_{12}, n_{23}, n_{31}; \alpha_1, \alpha_2, \alpha_3) \\ &= \int r_1^{n_1-1} r_2^{n_2-1} r_3^{n_3-1} r_{12}^{n_{12}-1} r_{23}^{n_{23}-1} r_{31}^{n_{31}-1} \\ &\quad \times \exp(-\alpha_1 r_1 - \alpha_2 r_2 - \alpha_3 r_3) d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3. \end{aligned} \tag{4}$$

Consider the following "generating" integral,

$$\begin{aligned} &\tilde{I}(\alpha_1, \alpha_2, \alpha_3) \\ &= \int \frac{\exp(-\alpha_1 r_1 - \alpha_2 r_2 - \alpha_3 r_3)}{r_1 r_2 r_3 r_{12} r_{23} r_{31}} d^3\mathbf{r}_1 d^3\mathbf{r}_2 d^3\mathbf{r}_3. \end{aligned} \tag{5}$$

E. Remiddi (PRA,**44**,9(1991)) derived a closed-form formula of the above integral

$$
\begin{aligned}
&\tilde{I}(\alpha_1, \alpha_2, \alpha_3) \\
=&\frac{32\pi^3}{\alpha_1\alpha_2\alpha_3}\Big\{ \ln\Big[\frac{\alpha_1+\alpha_2}{\alpha_3}\Big]\ln\Big[\frac{\alpha_1+\alpha_2+\alpha_3}{\alpha_1+\alpha_2}\Big] - \mathrm{Li}_2\Big[-\frac{\alpha_3}{\alpha_1+\alpha_2}\Big] \\
&- \mathrm{Li}_2\Big[1-\frac{\alpha_3}{\alpha_1+\alpha_2}\Big] + \ln\Big[\frac{\alpha_3+\alpha_1}{\alpha_2}\Big]\ln\Big[\frac{\alpha_1+\alpha_2+\alpha_3}{\alpha_3+\alpha_1}\Big] \\
&- \mathrm{Li}_2\Big[-\frac{\alpha_2}{\alpha_3+\alpha_1}\Big] - \mathrm{Li}_2\Big[1-\frac{\alpha_2}{\alpha_3+\alpha_1}\Big] \\
&+ \ln\Big[\frac{\alpha_2+\alpha_3}{\alpha_1}\Big]\ln\Big[\frac{\alpha_1+\alpha_2+\alpha_3}{\alpha_2+\alpha_3}\Big] \\
&- \mathrm{Li}_2\Big[-\frac{\alpha_1}{\alpha_2+\alpha_3}\Big] - \mathrm{Li}_2\Big[1-\frac{\alpha_1}{\alpha_2+\alpha_3}\Big]\Big\}.
\end{aligned}
$$

The closed-form result for the integral (4) with $n_1 = 1$, $n_2 = 1$, $n_3 = 1$, $n_{12} = 2$, $n_{23} = 0$ and $n_{31} = 2$ was also derived in Remiddi's paper.

With the closed-form expression for $\tilde{I}(\alpha_1, \alpha_2, \alpha_3)$, one can easily derive that

$$\tilde{J}(n_1, n_2, n_3, 0, 0, 0) = \left(-\frac{\partial}{\partial \alpha_1}\right)^{n_1} \left(-\frac{\partial}{\partial \alpha_2}\right)^{n_2} \left(-\frac{\partial}{\partial \alpha_3}\right)^{n_3} \times \tilde{I}(\alpha_1, \alpha_2, \alpha_3). \tag{6}$$

Now a series of questions arise:

- Can it produce the expression for the general integral $\tilde{J}(n_1, n_2, n_3, n_{12}, n_{23}, n_{31})$ with $n_{12}$, $n_{23}$, $n_{31}$ being arbitrary nonnegative integers?
- And how?

$$\tilde{J}(n_1, n_2, n_3 + 1, n_{12}, n_{23}, n_{31})$$
$$= \frac{1}{\alpha_1\alpha_2\alpha_3}\Big\{(n_{23} - 1)n_{23}n_1\tilde{J}(n_1 - 1, n_2 + 1, n_3, n_{12}, n_{23} - 2, n_{31})$$
$$+ (n_{31} - 1)n_{31}n_2\tilde{J}(n_1 + 1, n_2 - 1, n_3, n_{12}, n_{23}, n_{31} - 2)$$
$$- (n_{12} - 1)n_{12}n_1\tilde{J}(n_1 - 1, n_2 - 1, n_3, n_{12}, n_{23}, n_{31}) + \cdots\Big\}. \tag{7}$$

Two other recursions for $\tilde{J}(n_1 + 1, n_2, n_3, n_{12}, n_{23}, n_{31})$ and $\tilde{J}(n_1, n_2 + 1, n_3, n_{12}, n_{23}, n_{31})$ can be obtained by symmetry.

$$
\begin{aligned}
&\tilde{J}(0,0,0,n_{12}+2,n_{23},n_{31}) \\
&\quad = \frac{1+n_{12}}{2}\Big\{\frac{1}{\alpha_1^2}\Big[\frac{(n_{31}-1)n_{31}}{1+n_{12}}\tilde{J}(0,0,0,n_{12}+2,n_{23},n_{31}-2) \\
&\quad + (n_{12}+n_{23}+2n_{31})\tilde{J}(0,0,0,n_{12},n_{23},n_{31}) \\
&\quad + \frac{(n_{31}-1)n_{31}}{1+n_{23}}\tilde{J}(0,0,0,n_{12}+2,n_{23},n_{31}-2)+\cdots\Big] \\
&\quad + \frac{1}{\alpha_2^2}\Big[\cdots\Big] - \frac{\alpha_3^2}{\alpha_1^2\alpha_2^2}\Big[\cdots\Big]\Big\}.
\end{aligned} \tag{8}
$$

Two other recursions for $\tilde{J}(0,0,0,n_{12},n_{23}+2,n_{31})$ and $\tilde{J}(0,0,0,n_{12},n_{23},n_{31}+2)$ can be obtained by symmetry.

Using the recursions given above, the boundary terms and some other conditions, one can evaluate the integral $\tilde{J}(n_1, n_2, n_3, n_{12}, n_{23}, n_{31})$ analytically.

(M. Puchalski, K. Pachucki and E. Remiddi, PRA **70**, 032502 (2004))

Furthermore, by introducing and developing some numerical methods, some evaluations for relativistic corrections are obtained.

(K. Pachucki et al, PRA **71**, 032514 (2005); K. Puchalski et al, PRA **73**, 022503 (2006))

# Fromm-Hill integral

An analytic expression for the generating integral (2) is given by (D. M. Fromm and R. N. Hill, PRA **36**, 3(1987))

$$I(\alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31}) = \frac{16\pi^3}{\sigma}\left[\sum_{j=1}^{3} u(\beta_0^{(0)}\beta_0^{(j)}) + \sum_{j=0}^{3}\sum_{k=0}^{3} v(\gamma_k^{(j)}/\sigma)\right], \qquad (9)$$

where $u(z) = \mathrm{Li}_2(z) - \mathrm{Li}_2(1/z)$ and

$$v(z) = \frac{1}{2}\mathrm{Li}_2\left[\frac{1}{2}(1-z)\right] + \frac{1}{4}\ln^2\left[\frac{1}{2}(1+z)\right] - \frac{1}{2}\mathrm{Li}_2\left[\frac{1}{2}(1+z)\right] - \frac{1}{4}\ln^2\left[\frac{1}{2}(1-z)\right]$$

with $\mathrm{Li}_2(z)$ the dilogarithm function, defined by

$$\mathrm{Li}_2(z) = -\int_0^z \xi^{-1}\ln(1-\xi)d\xi.$$

The quantity $\sigma$ is the square root of a homogeneous six-degree polynomial in the $\alpha$'s:

$$\sigma = \Big[\alpha_1^2\alpha_{23}^2(\alpha_1^2 - \alpha_2^2 - \alpha_3^2 - \alpha_{12}^2 + \alpha_{23}^2 - \alpha_{31}^2)
+ \alpha_2^2\alpha_{31}^2(-\alpha_1^2 + \alpha_2^2 - \alpha_3^2 - \alpha_{12}^2 - \alpha_{23}^2 + \alpha_{31}^2)
+ \alpha_3^2\alpha_{12}^2(-\alpha_1^2 - \alpha_2^2 + \alpha_3^2 + \alpha_{12}^2 - \alpha_{23}^2 - \alpha_{31}^2)
+ \alpha_1^2\alpha_2^2\alpha_3^2 + \alpha_1^2\alpha_{12}^2\alpha_{31}^2 + \alpha_2^2\alpha_{23}^2\alpha_{12}^2 + \alpha_3^2\alpha_{31}^2\alpha_{23}^2\Big]^{1/2}.$$

The $\gamma_k^{(j)}$ $(k, j = 0, 1, 2, 3)$ are homogeneous third-degree polynomials in the $\alpha$'s, and $\beta_k^{(j)}$ is defined by

$$\beta_k^{(j)} = (\sigma - \gamma_k^{(j)})/(\sigma + \gamma_k^{(j)}).$$

Caution 1:

The functions $u$ and $v$ are multiple valued,
the formula (9) holds only if the branches of them are chosen correctly.

| Function | Branch points |
|---|---|
| $\ln(z)$ | $0, \quad \infty$ |
| $\mathrm{Li}_2(z)$ | $1, \quad \infty$ |
| $u(z)$ | $0, \quad 1, \quad \infty$ |
| $v(z)$ | $1, \quad -1, \quad \infty$ |

If the branch cut for the logarithm is taken to run from 0 to $\infty$ along the negative real axis and the principal branch is chosen as

$$\ln(z) = \ln|z| + i\arg(z), \qquad -\pi < \arg(z) < \pi,$$

then the branch cuts and the principal branches for $\mathrm{Li}_2(z)$, $u(z)$ and $v(z)$ are determined.

The singularities of the expression (9) may occur at

$$\sigma = 0,$$

$$(\gamma_k^{(j)})^2 - \sigma^2 = 0 \qquad \text{for} \qquad k, j = 0, 1, 2, 3$$

and

$$\gamma_k^{(k)} + \gamma_k^{(0)} = 0 \qquad \text{for} \qquad k \neq 0.$$

There are 20 cases should be considered!

- True sigularities **VS.** Cancelling singularities

Luckily, the situations for singularities may be reduced to

$$\sigma = 0,$$

$$\begin{cases} -\alpha_1 + \alpha_2 + \alpha_3 = 0, \\ \alpha_1 - \alpha_2 + \alpha_3 = 0, \\ \alpha_1 + \alpha_2 - \alpha_3 = 0, \end{cases}$$

$$\begin{cases} -\alpha_1 + \alpha_{12} + \alpha_{31} = 0, \\ \alpha_1 - \alpha_{12} + \alpha_{31} = 0, \\ \alpha_1 + \alpha_{12} - \alpha_{31} = 0, \end{cases}$$

$$\begin{cases} -\alpha_2 + \alpha_{23} + \alpha_{12} = 0, \\ \alpha_2 - \alpha_{23} + \alpha_{12} = 0, \\ \alpha_2 + \alpha_{23} - \alpha_{12} = 0, \end{cases}$$

and

$$\begin{cases} -\alpha_3 + \alpha_{31} + \alpha_{23} = 0, \\ \alpha_3 - \alpha_{31} + \alpha_{23} = 0, \\ \alpha_3 + \alpha_{31} - \alpha_{23} = 0. \end{cases}$$

Three obstacles appear when applying the closed-form formula (9) to generate the basic integral $J(n_1, n_2, n_3, n_{12}, n_{23}, n_{31}; \alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31})$:

- determine the correct branches of $u$ and $v$
- remove the canceling singularities analytically
- differentiate over the $\alpha$'s, especially at the canceling singularities

The corresponding solving methods:

- Branch tracking
- Use some analytic techniques
- Develop a new recursive relations for the differentials

- Branch tracking

Consider the path $(1, 1, 1, \lambda, \lambda, \lambda)(0 \leq \lambda \leq 1)$ which runs from SRP $(1, 1, 1, 1, 1, 1)$ to ARP $(1, 1, 1, 0, 0, 0)$.

The correct expression for $I$ around SRP is given by

$$\begin{aligned} I(1, 1, 1, \lambda, \lambda, \lambda) =& 16\pi^3 (1 - 3\lambda^2)^{-1/2} \\ & \times \left[ v(z_1(\lambda)) + 3v(z_2(\lambda)) + 3v(z_3(\lambda)) \right. \\ & \left. + 9v(z_4(\lambda)) + 3u(z_5(\lambda)) \right] \end{aligned}$$

with the choices of the principal branches of $u$ and $v$ and the square root being positive imaginary.

Over the straight-line path from $\lambda = 1$ to $\lambda = 0$, there are two canceling singular points at $\lambda = \frac{1}{\sqrt{3}}$ and $\lambda = \frac{1}{2}$, so the following modified path will be used in the tracking

$$
\begin{aligned}
\lambda &= x, & 1 \geq x \geq \tfrac{1}{\sqrt{3}} + \delta, \\
\lambda &= \tfrac{1}{\sqrt{3}} + \delta e^{i\theta}, & -\pi \leq \theta \leq 0, \\
\lambda &= x, & \tfrac{1}{\sqrt{3}} - \delta \geq x \geq \tfrac{1}{2} + \delta, \\
\lambda &= \tfrac{1}{2} + \delta e^{i\theta}, & -\pi \leq \theta \leq 0, \\
\lambda &= x, & \tfrac{1}{2} - \delta \geq x \geq 0,
\end{aligned}
$$

where $\delta$ is a small positive real number.

After the complicated tracking, we find the correct expression of $I$ at ARP

$$\begin{aligned} & I(1,1,1,\lambda,\lambda,\lambda) \\ & = 16\pi^3(1-3\lambda^2)^{-1/2} \lim_{\epsilon\to 0_+} \left\{ -\pi^2 - i\pi \ln\left[\frac{1+z_1(\lambda)}{1-z_1(\lambda)}\right] \right. \\ & \quad + v(z_1(\lambda)) + 3v(z_2(\lambda)-i\epsilon) + 3v(z_3(\lambda)+i\epsilon) \\ & \quad \left. + 9v(z_4(\lambda)) + 3u(z_5(\lambda)) \right\} \end{aligned}$$

with also the choices of the principal branches of $u$ and $v$, and the square root now, changing to be positive real.

Hence the value of $I(\alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31})$ in the neighborhood of ARP is given by

$$I(\alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31})$$

$$= \frac{16\pi^3}{\sigma} \lim_{\epsilon \to 0_+} \left\{ -\pi^2 - i\pi \ln \left[ \frac{1 + \gamma_0^{(0)}/\sigma}{1 - \gamma_0^{(0)}/\sigma} \right] + \sum_{j=1}^{3} u(\beta_0^{(0)} \beta_0^{(j)}) \right.$$

$$+ v(\gamma_0^{(0)}/\sigma) + \sum_{j=1}^{3} v(\gamma_j^{(j)}/\sigma - i\epsilon) + \sum_{j=1}^{3} v(\gamma_0^{(j)}/\sigma + i\epsilon)$$

$$\left. + \sum_{j=0}^{3} \sum_{\substack{k=1 \\ k \neq j}}^{3} v(\gamma_k^{(j)}/\sigma) \right\}.$$

We consider the general case, which tracks from the SRP $(1,1,1,1,1,1)$ to an arbitrary one $(\alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31})$:

- Step 1: Consider the path $((\alpha_1 - 1)\lambda + 1, 1, 1, 1, 1, 1)$, where $\lambda$ runs from $\lambda = 0$ to $\lambda = 1$ and this means we track from $(1,1,1,1,1,1)$ to $(\alpha_1, 1, 1, 1, 1, 1)$.
- Step 2: Consider the path $(\alpha_1, (\alpha_2 - 1)\lambda + 1, 1, 1, 1, 1), \ldots$

$$\vdots$$

- Step 6: Consider the path $(\alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, (\alpha_{31} - 1)\lambda + 1)$, which means tracking from $(\alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, 1)$ to $(\alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31})$.

We should point out here that, using some mathematical techniques can simplify the whole tracking process to some extent. But it is still incredibly complicated.

For a point

$$(\alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31}) = (872, 78.08, 34.09, 12, 12.788, 10.34),$$

the correct expression of $I$ around this point is

$$
\begin{aligned}
I(&\alpha_1,\alpha_2,\alpha_3,\alpha_{12},\alpha_{23},\alpha_{31}) \\
&= \frac{16\pi^3}{\sigma} \lim_{\epsilon\to 0_+} \Bigg\{ \\
&u(\beta_0^{(0)}\beta_0^{(1)} + i\epsilon) + u(\beta_0^{(0)}\beta_0^{(2)}) + u(\beta_0^{(0)}\beta_0^{(3)}) \\
&+ \sum_{j=0}^{1}\sum_{k=0}^{3} v(\gamma_k^{(j)}/\sigma) + v(\gamma_0^{(2)}/\sigma - i\epsilon) + v(\gamma_1^{(2)}/\sigma + i\epsilon) \\
&+ v(\gamma_2^{(2)}/\sigma + i\epsilon) + v(\gamma_3^{(2)}/\sigma + i\epsilon) + v(\gamma_0^{(3)}/\sigma + i\epsilon) \\
&+ v(\gamma_1^{(3)}/\sigma - i\epsilon) + v(\gamma_2^{(3)}/\sigma + i\epsilon) + v(\gamma_3^{(3)}/\sigma + i\epsilon)
\end{aligned}
$$

$$-i\pi\ln\left[\frac{1+\gamma_0^{(0)}/\sigma}{1-\gamma_0^{(0)}/\sigma}\right]+i\pi\ln\left[\frac{1+\gamma_1^{(0)}/\sigma}{1-\gamma_1^{(0)}/\sigma}\right]+2i\pi\ln\left[\frac{1+\gamma_2^{(0)}/\sigma}{1-\gamma_2^{(0)}/\sigma}\right]$$

$$-i\pi\ln\left[\frac{1+\gamma_0^{(1)}/\sigma}{1-\gamma_0^{(1)}/\sigma}\right]+i\pi\ln\left[\frac{1+\gamma_2^{(1)}/\sigma}{1-\gamma_2^{(1)}/\sigma}\right]+i\pi\ln\left[\frac{1+\gamma_3^{(1)}/\sigma}{1-\gamma_3^{(1)}/\sigma}\right]$$

$$+i\pi\ln\left[\frac{1+\gamma_0^{(2)}/\sigma}{1-\gamma_0^{(2)}/\sigma}\right]+i\pi\ln\left[\frac{1+\gamma_2^{(2)}/\sigma}{1-\gamma_2^{(2)}/\sigma}\right]-i\pi\ln\left[\frac{1+\gamma_3^{(2)}/\sigma}{1-\gamma_3^{(2)}/\sigma}\right]$$

$$-i\pi\ln\left[\frac{1+\gamma_0^{(3)}/\sigma}{1-\gamma_0^{(3)}/\sigma}\right]-2i\pi\ln\left[\frac{1+\gamma_3^{(2)}/\sigma}{1-\gamma_3^{(2)}/\sigma}\right]\quad-\quad\pi^2\Bigg\},$$

and

$$I(872, 78.08, 34.09, 12, 12.788, 10.34)$$
$$= 5.272897938711298\times 10^{-4}.$$

| $\lambda$ | $I(1,1,1,\lambda,\lambda,\lambda)$ |
|---|---|
| 0.05 | $3.63236729624140 \times 10^2$ |
| 0.15 | $2.59682121353657 \times 10^2$ |
| 0.25 | $1.93536770465417 \times 10^2$ |
| 0.45 | $1.17605235633348 \times 10^2$ |
| 0.70 | $7.08583266363307 \times 10$ |
| 0.95 | $4.65491345483885 \times 10$ |
| 1.00 | $4.31360835924724 \times 10$ |

# The future(ongoing) work

- To calculate $J(n_1, n_2, n_3, n_{12}, n_{23}, n_{31}; \alpha_1, \alpha_2, \alpha_3, \alpha_{12}, \alpha_{23}, \alpha_{31})$
- The relativistic and QED corrections
- The five-body problems

*THANK YOU SO MUCH FOR YOUR ATTENTION!*