

NONPERTURBATIVE EFFECTS FOR SOME MODELS OF QUANTUM SYSTEMS

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**The Actual Problems of Microworld Physics
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KEY POINTS

- **Basics of conventional perturbation theory (CPT) – small parameter and adiabatic switch-off interaction**
- **What is nonperturbative (NPT) , uniformly suitable estimation (USE) of zero approximation?**
- **Quantum anharmonic oscillator (QAO): example for main ideas of the method**
- **Regularization of the Coulomb scattering cross section**
- **Example for the quantum field theory**

What is NPT and USE? (1)

1. Usual perturbation theory (PT) is based on use of some small real physical parameter!

$$H = H_0 + \lambda V$$

$$H |\Psi_n\rangle = E_n(\lambda) |\Psi_n\rangle$$

2. PT is asymptotical in the most cases, that is eigenvalues and eigenfunctions can be calculated approximately only in small range of physical parameter and quantum numbers n !

$$\begin{aligned} \lambda \ll 1, & \quad - \text{weak coupling} \\ \lambda \gg 1, & \quad - \text{strong coupling} \\ (\lambda' = \lambda^{-1}) \end{aligned}$$

3. PT is based on adiabatic switch-off of the interaction

What is NPT and USE? (2)

1. NPT means that some **artificial (numerical) parameter** is used for approximate solution of the Schrodinger equation (1) and the calculation method should be **universal for any Hamiltonian!**

Simple example: numerical solution of the differential equation with the step of the finite-difference approximation as the parameter

2. USE means that the approximate solution of (1) should be suitable in the **whole range** of the physical parameters of Hamiltonian and for all **quantum numbers!**

$$\frac{|E_n^{(0)}(\lambda) - E_n^{(ex)}(\lambda)|}{E_n^{(ex)}(\lambda)} < \xi^{(0)}$$

3. Sequential approximations **converge** to the exact solution

$$\lim_{s \rightarrow \infty} E_n^{(s)}(\lambda) = E_n^{(ex)}(\lambda)$$

Formal scheme of perturbation series

$$|\psi_n\rangle = \lim_{\alpha \rightarrow 0} \frac{\hat{U}_\alpha |n\rangle}{\langle n | \hat{U}_\alpha |n\rangle}, \quad E_n = E_n^{(0)} + \lim_{\alpha \rightarrow 0} \frac{\langle n | \hat{H}_1 \hat{U}_\alpha |n\rangle}{\langle n | \hat{U}_\alpha |n\rangle}$$

$$\hat{U}_\alpha = 1 + \sum_{s=1}^{\infty} \frac{1}{E_n^{(0)} - \hat{H}_0 + is\alpha} \hat{H}_1 \frac{1}{E_n^{(0)} - \hat{H}_0 + i(s-1)\alpha} \hat{H}_1 \dots$$

successive approximations are defined by the operator powers

$$\hat{B}_n = \frac{1}{E_n^{(0)} - \hat{H}_0} \hat{H}_1,$$

$$\hat{H} = \hat{H}_0 + \hat{H}_1,$$

Example 1: QAO - How operator method (OM) leads to NPT and USE (1)

PT: $\hat{H}'_0 = \frac{1}{2} (2\hat{n} + 1), \quad \hat{n} = a^+ a, \quad \hat{H}'_1 = \frac{\lambda}{4} (a + a^+)^4,$

$\|\hat{B}_n^{\text{PT}}\| = c\lambda k \quad (c = \text{const}),$ PT series diverges as factorial for any λ

OM:

$$\hat{H}_0 = \frac{1}{4\omega^2} [\omega(\omega^2 + 1)(2\hat{n} + 1) + 3\lambda(2\hat{n}^2 + 2\hat{n} + 1)],$$

$$\hat{H}_1 = \frac{1}{4\omega^2} a^{+2} [2\lambda(2\hat{n}^2 + 3) - \omega(\omega^2 - 1)]$$

$$+ \frac{1}{4\omega^2} [2\lambda(2\hat{n} + 3) - \omega(\omega^2 - 1)] a^2 + \frac{\lambda}{4\omega^2} (a^{+4} + a^4).$$

$\|\hat{B}_n^{\text{OM}}\| < \frac{2}{3},$ OM series converges as geometric series for any λ

QAO: How operator method (OM) leads to NPT and USE (2)

$$E_n(\lambda) - ?$$

P T zero approximation:

$$E_n^{(PT)} = \langle n | H_0 | n \rangle = \left(n + \frac{1}{2}\right)$$

O M zero approximation:

$$E_n^{(OM)}(\omega, \lambda) = \langle n, \omega | H | n, \omega \rangle$$

Exact condition

$$E_n^{(0)}(\omega, \lambda) = \frac{1}{4\omega} (\omega^2 + 1)(1 + 2n) + \frac{3\lambda}{4\omega^2} (1 + 2n + 2n^2)$$

$$\frac{\partial E_n(\lambda)}{\partial \omega} = 0 \Rightarrow \frac{\partial E_n^{(OM)}(\lambda)}{\partial \omega} = 0$$

$$\omega_n^3 - \omega_n - 6\lambda \frac{1 + 2n + 2n^2}{1 + 2n} = 0.$$

$$E_n^{(0)}(\lambda) = \frac{1}{4} \left(3\omega_n + \frac{1}{\omega_n} \right) \left(n + \frac{1}{2} \right)$$

QAO: How operator method (OM) leads to NPT and USE (3)

USE for OM means:

Weak coupling

$$E_n^{(0)}(\lambda) = n + \frac{1}{2} + \frac{3}{4} \lambda(1 + 2n + 2n^2) - \frac{9}{4} \lambda^2 \frac{(1 + 2n + 2n^2)^2}{1 + 2n} + \frac{27}{2} \lambda^3 \frac{(1 + 2n + 2n^2)^3}{(1 + 2n)^2} + O(\lambda^4).$$

Strong coupling

$$E_n(\lambda) = \lambda^{1/3} \left[\frac{3^{4/3}}{2^{8/3}} (1 + 2n + 2n^2)^{1/3} (1 + 2n)^{2/3} + \frac{1}{4 \cdot 6^{1/3}} \frac{(1 + 2n)^{4/3}}{(1 + 2n + 2n^2)^{1/3}} \frac{1}{\lambda^{2/3}} - \frac{1}{144} \frac{(2n + 1)^2}{(1 + 2n + 2n^2)} \frac{1}{\lambda^{4/3}} + O\left(\frac{1}{\lambda^2}\right) \right]$$

Comparison of Some Numerical and OM Zeroth Approximation Results for QAO

$E_n^{(T)} (E_n^{(OM)})$	λ			
	0.1	1	10	100
$n = 0$	0.560307 (0.559146)	0.812500 (0.803771)	1.53125 (1.50497)	3.19244 (3.13138)
$n = 10$	17.26588 (17.35190)	32.66349 (32.93326)	68.17094 (68.03695)	145.8383 (147.2270)
$n = 40$	94.84034 (95.56017)	192.7883 (194.6022)	409.8935 (413.9383)	880.546 (889.325)

QAO: How operator method (OM) leads to NPT and USE (4)

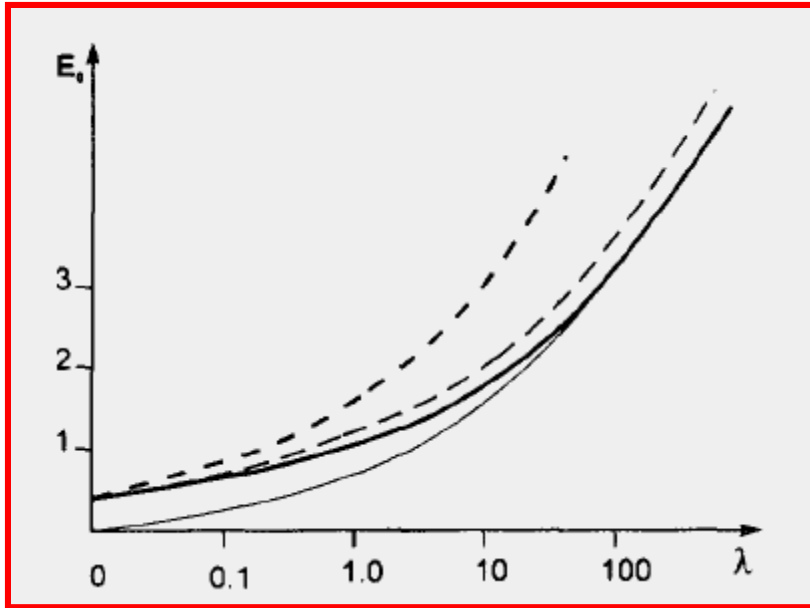
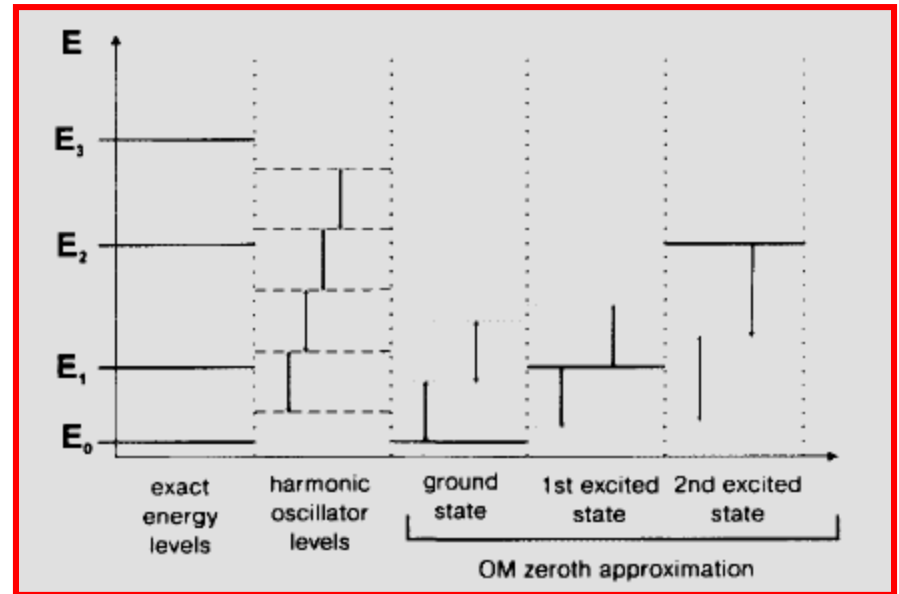


FIG. 2. Comparison of the function $E_0(\lambda)$ with its different approximations: — exact; — strong coupling; --- PT; - - - OM zeroth approximation.

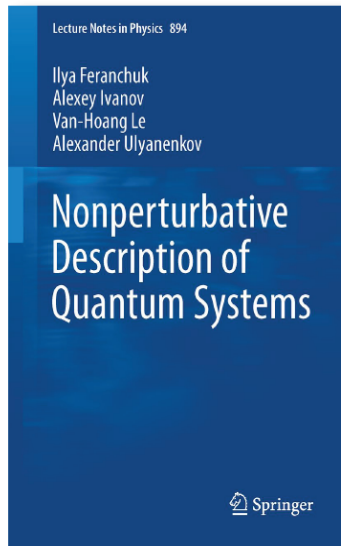
**OM gives the local approximation
for each level !**



A lot of other examples and cited publication in the book



[springer.com](https://www.springer.com)



2015, 380 p. 62 illus. in color.

 Printed book

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Nonperturbative Description of Quantum Systems

Series: Lecture Notes in Physics, Vol. 894

- ▶ Gives a detailed introduction and comprehensive description of non-perturbative operator method
- ▶ Provides an extended review of other non-perturbative methods for description of quantum systems
- ▶ Displays numerous applications of operator method for various problems of theoretical physics

This book introduces systematically the operator method for the solution of the Schrödinger equation. This method permits to describe the states of quantum systems in the entire range of parameters of Hamiltonian with a predefined accuracy. The operator method is unique compared with other non-perturbative methods due to its ability to deliver in zeroth approximation the uniformly suitable estimate for both ground and excited states of quantum system. The method has been generalized for the application to quantum statistics and quantum field theory. In this book, the numerous applications of operator method for various physical systems are demonstrated. Simple models are used to illustrate the basic principles of the method which are further used for the solution of complex problems of quantum theory for many-particle systems. The results obtained are supplemented by numerical calculations, presented as tables and figures.

Example 2: Coulomb scattering

Problems of the asymptotic theory

$$\psi(\mathbf{r}) = \left[e^{i\mathbf{p}\mathbf{r}} + \hat{f}(\mathbf{p}, \mathbf{p}') \frac{e^{i\mathbf{p}'\mathbf{r}}}{r} \right] u(\mathbf{p}); \quad \mathbf{p}' = p \frac{\mathbf{r}}{r}$$

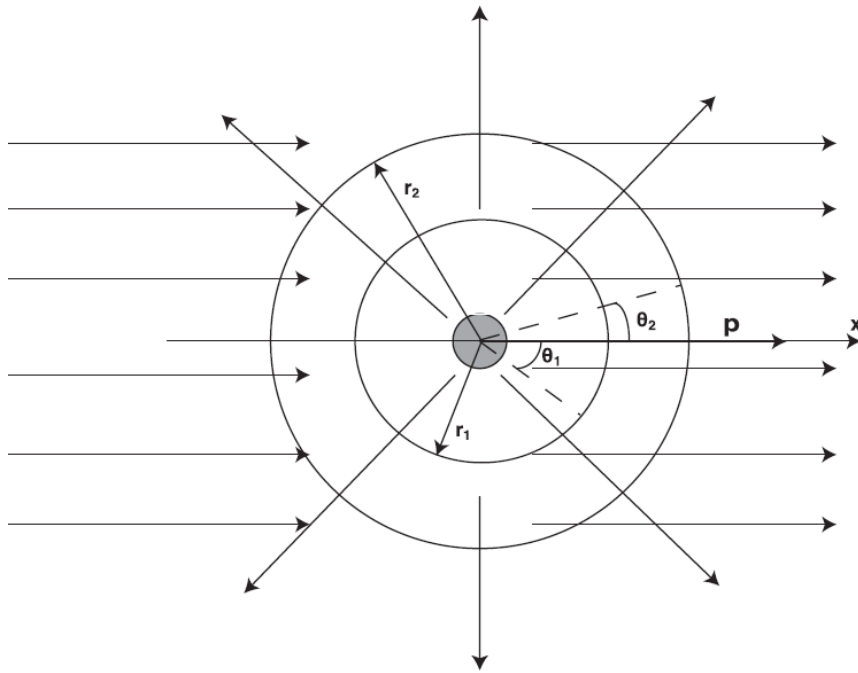
$$\frac{d\sigma}{d\Omega} = \left(\frac{Z\alpha}{2pv} \right)^2 \left(1 - v^2 \sin^2 \frac{\theta}{2} \right) \frac{1}{\sin^4 \frac{\theta}{2}}$$

$$\sigma_{\text{tot}} = \int d\sigma(\theta), \quad \sigma_{\text{tr}} = \int (1 - \cos \theta) d\sigma(\theta)$$

Scattering flux exceeds the incident flux ??

Exact wave function has no singularity!

Characteristic parameters of the problem



$$pr - \mathbf{p} \cdot \mathbf{r} = 2pr \sin^2(\theta/2) > 1$$

$$\theta > \theta_0 \equiv \sqrt{\frac{2}{pr}}$$

Boundary of the wave zone

$$N_{\text{int}} = 2\pi j_0 \int_0^{\theta_0} \frac{d\sigma(\theta)}{d\Omega} \sin\theta d\theta \simeq \pi j_0 \sigma(0) \theta_0^2 \simeq 2\pi \frac{j_0 \sigma(0)}{pr}$$

$$N_{\text{int}}^C = 2\pi j_0 \int_{\theta_{\text{min}}}^{\theta_0} \frac{d\sigma(\theta)}{d\Omega} \sin\theta d\theta \simeq 4\pi j_0 \left(\frac{Z\alpha}{pv}\right)^2 \frac{1}{\theta_{\text{min}}^2}$$

$$\theta_0 > \theta_{\text{min}}$$

$$\theta_{\text{min}} \simeq \frac{a}{r}, \quad a \simeq \frac{1}{\Delta p} \quad N_{\text{int}}^C \simeq 2\pi j_0 \left(\frac{Z\alpha}{v}\right)^2 r^2 \left(\frac{1}{pa}\right)^2 \simeq 2\pi j_0 \left(\frac{Z\alpha}{v}\right)^2 r^2 \left(\frac{\Delta p}{p}\right)^2$$

Angular size of the incident beam $\theta_{\text{min}} < \theta_0, \quad \frac{2pa^2}{r} < 1 \quad \frac{pa^2}{r} \frac{p^2}{m^2} > 1$

Nonexistence of the conventional Born series

$$\psi^{(1)} = -\frac{1}{4\pi}(\boldsymbol{\gamma} \cdot \boldsymbol{\nabla} - \gamma_4 \varepsilon - m)\gamma_4 u \int \frac{e^{ip|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \frac{Z\alpha}{r'} e^{i\mathbf{p}\cdot\mathbf{r}} d\mathbf{r}' \quad (10)$$

$$I(\mathbf{r}) = \frac{ie^{i\mathbf{p}\cdot\mathbf{r}}}{2p} \int_0^1 du \frac{e^{i(pr-\mathbf{p}\cdot\mathbf{r})u}}{u}$$

This wave function doesn't exist at any angles !

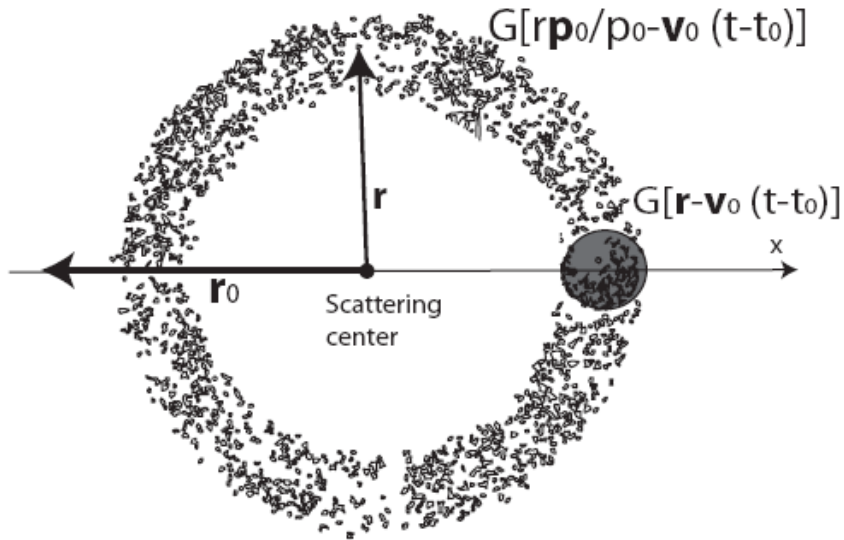
Regularization is possible and similar to the infrared regularization

G. Gasaneo and L. U. Ancarani, *Phys. Rev. A* **80**, 062717 (2009).

$$\Psi^{(1)} = f_B(\theta) \frac{e^{ipr}}{r} + \Delta\Psi^{(1)}; \quad \Psi^{(2)} = -\Delta\Psi^{(1)} + \Delta\Psi^{(2)}$$

Total regularization includes all terms of Born series and depends on the angle !

Non-asymptotic time-dependent scattering theory



$$\Psi^\pm(\mathbf{r}) = C^\pm e^{i\mathbf{p}\mathbf{r}} \left(1 - \frac{i\alpha\nabla}{2\varepsilon} \right) \times$$

$$F[\pm i\xi, 1, i\mathbf{p}\mathbf{r}(1 - \cos\theta)]u(\mathbf{p}),$$

$$u(\mathbf{p}) = \begin{pmatrix} \sqrt{\varepsilon + m}v \\ \sqrt{\varepsilon - m}(\boldsymbol{\sigma} \cdot \boldsymbol{\nu})v \end{pmatrix}$$

$$C^\pm = \Gamma(1 \mp i\xi)e^{\frac{\pi\xi}{2}}, \quad \xi = \frac{Z\alpha\varepsilon}{p}$$

$$\Psi(\mathbf{r}, 0) = \int e^{i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}_0)} G(\mathbf{p}) d\mathbf{p},$$

$$G(\mathbf{p}) = \frac{1}{(2\pi)^3} \int d\mathbf{r} \tilde{G}(\mathbf{r}) e^{-i(\mathbf{p} - \mathbf{p}_0) \cdot \mathbf{r}}, \quad \int d\mathbf{r} |\tilde{G}(\mathbf{r})|^2 = 1 \quad (\xi)$$

$$\Psi(\mathbf{r}, t) = [\Phi(\mathbf{r}, t) + ip_0\Phi_1(\mathbf{r}, t)\boldsymbol{\alpha} \cdot (\mathbf{n} - \boldsymbol{\nu}_0)]u(\mathbf{p}_0);$$

$$\mathbf{n} = \frac{\mathbf{r}}{r}, \quad \boldsymbol{\nu}_0 = \frac{\mathbf{p}_0}{p_0};$$

$$\Phi(\mathbf{r}, t) = C \int F(i\xi, 1, iz)G(\mathbf{p}, t)d\mathbf{p};$$

$$\Phi_1(\mathbf{r}, t) = C \frac{\xi}{2\varepsilon(p_0)} \int F(i\xi + 1, 2, iz)G(\mathbf{p}, t)d\mathbf{p};$$

$$G(\mathbf{p}, t) = G(\mathbf{p})e^{-i\varepsilon(\mathbf{p})t + i\mathbf{p} \cdot (\mathbf{r} - \mathbf{r}_0)},$$

$$dI = (\mathbf{j} \cdot \mathbf{n})r^2 d\Omega,$$

$$\zeta' = Sp(\rho' \boldsymbol{\sigma}),$$

Analytical results

$$dI = 2p_0 Sp(T_1 \rho T_2^\dagger + T_2 \rho T_1^\dagger) r^2 d\Omega =$$

$$\left(|\Phi|^2 \mathbf{n} \cdot \boldsymbol{\nu}_0 + [2\varepsilon_0 \text{Im}(\Phi \Phi_1^*) - 2p_0^2 |\Phi_1|^2] (1 - \mathbf{n} \cdot \boldsymbol{\nu}_0) + \right.$$

$$\left. 2m \text{Re}(\Phi \Phi_1^*) \boldsymbol{\zeta} \cdot \boldsymbol{\tau} \right) r^2 d\Omega,$$

$$\boldsymbol{\tau} = \mathbf{n} \times \boldsymbol{\nu}_0, \quad \varepsilon_0 = \varepsilon(p_0).$$

$$\boldsymbol{\zeta}' = \frac{g\boldsymbol{\tau} + f\boldsymbol{\zeta} + c\boldsymbol{\zeta} \times \boldsymbol{\tau} + e\mathbf{n}(\boldsymbol{\tau}[\boldsymbol{\zeta} \times \boldsymbol{\nu}_0]) - e\mathbf{n} \times \boldsymbol{\tau}(\boldsymbol{\zeta} \cdot \boldsymbol{\nu}_0)}{f + g\boldsymbol{\zeta} \cdot \boldsymbol{\tau}}$$

$$g = 2m \text{Re}(\Phi \Phi_1^*);$$

$$f = |\Phi|^2 \mathbf{n} \cdot \boldsymbol{\nu}_0 + 2\varepsilon_0 \text{Im}(\Phi \Phi_1^*) (1 - \mathbf{n}_0 \cdot \boldsymbol{\nu}_0) -$$

$$2p_0^2 |\Phi_1|^2 (1 - \mathbf{n} \cdot \boldsymbol{\nu}_0);$$

$$c = |\Phi|^2 - 2\varepsilon_0 \text{Im}(\Phi \Phi_1^*) - 2p_0^2 |\Phi_1|^2;$$

$$e = 2p_0^2 |\Phi_1|^2 - 2(\varepsilon_0 - m) \text{Im}(\Phi \Phi_1^*).$$

Calculation of the cross-section (1)

Scattered flux can be separated from the incident one:

$$\frac{dI^{(1)}}{r^2 d\Omega} = \frac{2(\mathbf{n} \cdot \mathbf{p}_0)|C|^2}{|\Gamma(i\xi)|^2} \left| \int F(i\xi, 1, iz)G(\mathbf{p}, t)d\mathbf{p} \right|^2 \rightarrow$$

$$\frac{dI_{sc}^{(1)}}{r^2 d\Omega} = \frac{2(\mathbf{n} \cdot \mathbf{p}_0)|C|^2}{|\Gamma(i\xi)|^2} \left| \int U_1(i\xi, 1, iz)G(\mathbf{p}, t)d\mathbf{p} \right|^2.$$

After normalization on the incident wave packet flux

$$j_0 = \rho_0 \int \Psi_0^*(\mathbf{r})\alpha\Psi_0(\mathbf{r})d\mathbf{r}_0 =$$

$$\rho_0 \int |G(\mathbf{r} - \mathbf{r}_0)|^2 \bar{u}(\mathbf{p}_0)\alpha u(\mathbf{p}_0)d\mathbf{r}_0 = 2\mathbf{p}_0\rho_0,$$

differential cross-section can be calculated as $z = pr - \mathbf{p} \cdot \mathbf{r}$.

$$\frac{d\sigma^{(1)}}{d\Omega} = \frac{r^2}{j_0} \rho_0 \int d\mathbf{r}_0 \frac{dI_{sc}^{(1)}}{d\Omega} = (\mathbf{n} \cdot \boldsymbol{\nu}_0) \frac{|C|^2}{|\Gamma(i\xi)|^2} |U_1(i\xi, 1, iz_0)|^2 r^2.$$

Calculation of the cross-section (2)

$$\frac{d\sigma^{(2)}}{d\Omega} = \frac{r^2}{j_0} \rho_0 \int dr_0 \frac{dI_{sc}^{(2)}}{d\Omega} = \xi r^2 \times (1 - \mathbf{n} \cdot \boldsymbol{\nu}_0) |C|^2 \text{Im} \left[\frac{U_1(i\xi, 1, iz) U_1^*(i\xi + 1, 2, iz)}{\Gamma(i\xi) \Gamma^*(i\xi + 1)} \right];$$

$$\frac{d\sigma^{(3)}}{d\Omega} = \frac{r^2}{j_0} \rho_0 \int dr_0 \frac{dI_{sc}^{(3)}}{d\Omega} = r^2 \xi \frac{m}{\varepsilon_0} (\boldsymbol{\zeta} \cdot \boldsymbol{\tau}_0) |C|^2 \text{Re} \left[\frac{U_1(i\xi, 1, iz) U_1^*(i\xi + 1, 2, iz)}{\Gamma(i\xi) \Gamma^*(i\xi + 1)} \right].$$

$$\frac{d\sigma^{(4)}}{d\Omega} = -\frac{r^2}{2} \xi^2 v_0^2 (1 - \mathbf{n} \cdot \boldsymbol{\nu}_0) \times |C|^2 \left| U_1 \left[i\xi + 1, 2, i \left(\eta^2 + \frac{\tilde{\delta}^2}{2} \right) \right] \right|^2 \frac{1}{|\Gamma(i\xi + 1)|^2}.$$

$$\frac{d\sigma}{d\eta} = \frac{4\pi r}{p_0} \eta |C|^2 \left\{ \left(1 - \frac{\eta^2}{p_0 r} \right) \frac{|U_1(i\xi, 1, i\eta^2)|^2}{|\Gamma(i\xi)|^2} + \xi \frac{\eta^2}{p_0 r} \text{Im} \left[\frac{U_1(i\xi, 1, i\eta^2) U_1^*(i\xi + 1, 2, i\eta^2)}{\Gamma(i\xi) \Gamma^*(i\xi + 1)} \right] - \xi^2 \frac{\eta^2 v_0^2}{2 p_0 r} \frac{1}{|\Gamma(i\xi + 1)|^2} \left| U_1 \left[i\xi + 1, 2, i \left(\eta^2 + \frac{\tilde{\delta}^2}{2} \right) \right] \right|^2 \right\}$$

This part of the cross-section depends both from the distance and the wave vector at param

$$\theta = \theta_0 \eta = \eta \sqrt{\frac{2}{p_0 r}};$$

$$\frac{d\sigma}{d\eta} = \frac{4\pi r}{p_0} \xi^2 \left(1 - \frac{v_0^2 \eta^2}{2 p_0 r} \right) \frac{1}{\eta^3}$$

Mott formula in the same variables at small angles

Numerical results (1)

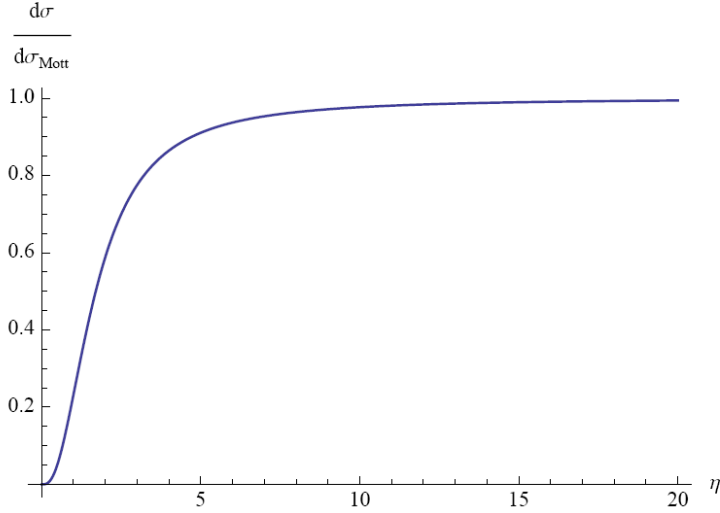


Figure 3: Comparison between the non-asymptotic cross section and the Mott cross section for the momentum $p_0 = 2 \cdot 10^{12} \text{ cm}^{-1}$, atomic number $Z = 80$, and a distance from the scattering center of $r = 100 \text{ cm}$, $\tilde{\delta} = 3$.

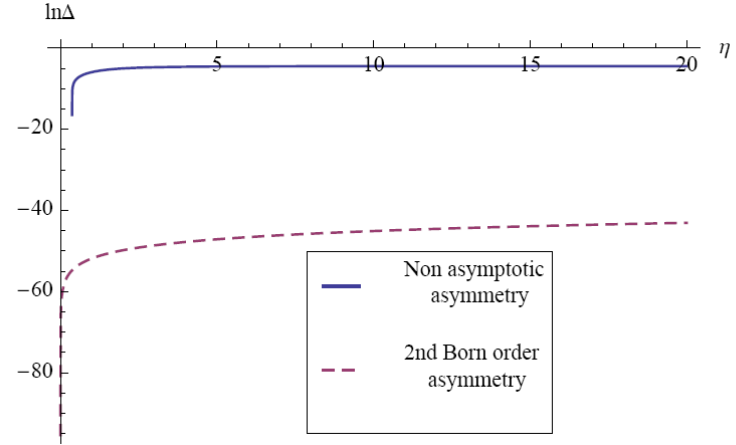


Figure 4: Comparison of the non-asymptotic asymmetry with the second order Born asymmetry for momentum $p_0 = 2 \cdot 10^{12} \text{ cm}^{-1}$, atomic number $Z = 80$, and a distance from the scattering center of $r = 100 \text{ cm}$, $\tilde{\delta} = 3$. Logarithmic scale has been used.

$$\sigma_{tot} = \frac{2\pi r}{p_0} \frac{|C|^2}{|\Gamma(i\xi)|^2} i_1(\xi) - \frac{2\pi}{p_0^2} \frac{|C|^2}{|\Gamma(i\xi)|^2} i_2(\xi) +$$

$$|C|^2 \frac{2\pi\xi}{p_0^2} \left(K_1 i_4(\xi) + K_2 i_3(\xi) \right) - \frac{\pi\xi^2 v_0^2}{p_0^2} \frac{|C|^2}{|\Gamma(i\xi + 1)|^2} i_5(\xi) +$$

$$\frac{2\pi|C|^2}{p_0^2} e^{-\pi\xi} \ln 2p_0 r \left(\xi K_2 - \frac{1}{|\Gamma(i\xi)|^2} - \frac{\xi^2 v_0^2}{2} \frac{1}{|\Gamma(i\xi + 1)|^2} \right).$$

$$\sigma_{tot}^{max} = 2\pi a^2 \frac{p_0^2}{m^2} f(\xi), \quad f(\xi) \leq 1,$$

Numerical results (2)

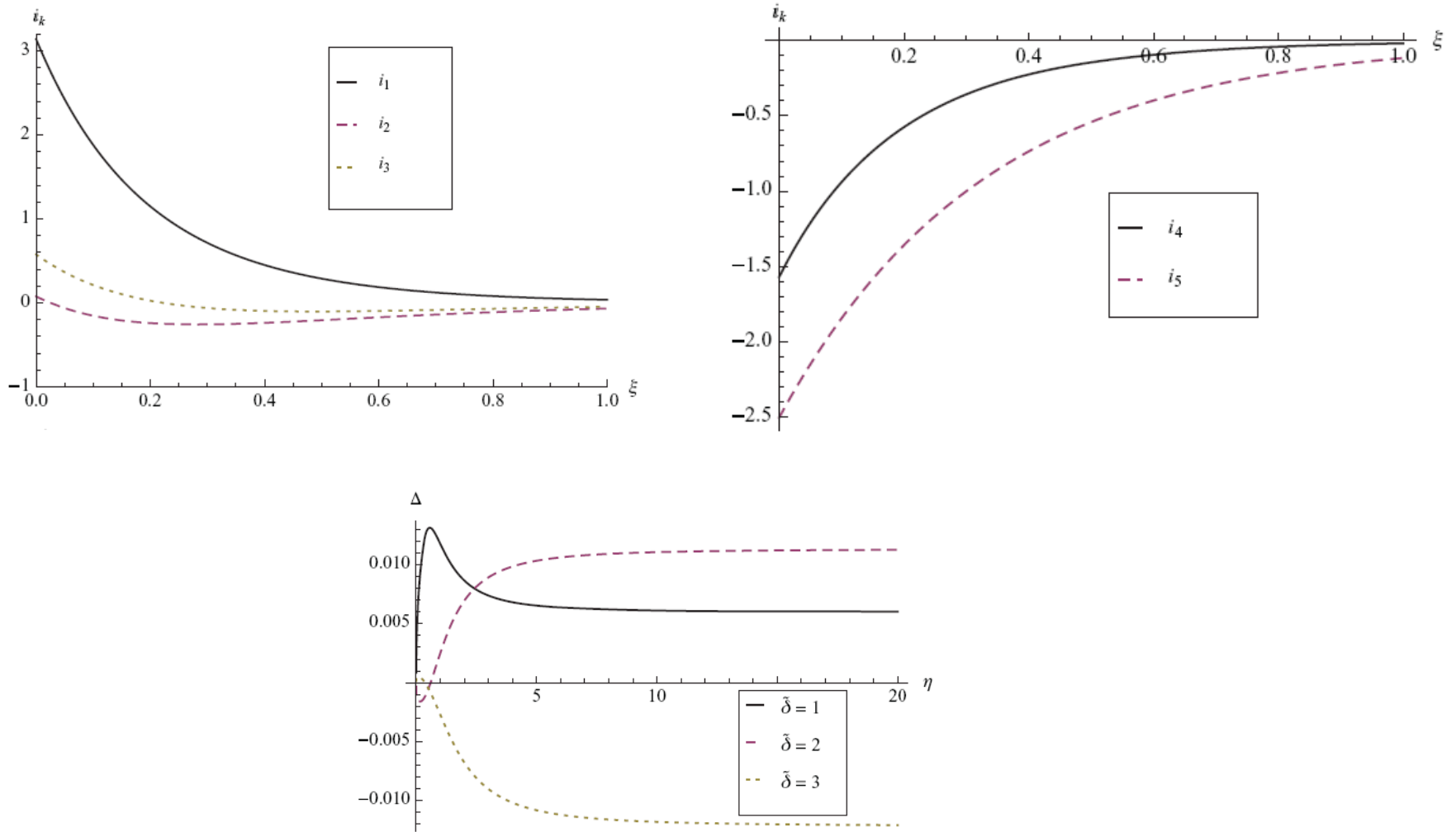


FIG. 5. (Color online) The asymmetry dependence on $\tilde{\delta}$ for momentum $p_0 = 2 \times 10^{12} \text{ cm}^{-1}$, atomic number $Z = 80$, and a distance from the scattering center of $r = 100 \text{ cm}$.

Publications:

1. V.G. Baryshevsky, L.N. Korennaya, I.D. Feranchuk

ZETP, 34, 249, 1972

Perturbation theory

2. V.G. Baryshevsky, I.D. Feranchuk, P.B. Kats

Phys.Rev.A 70, 052701 (2004)

Nonrelativistic case

3. I.D. Feranchuk, O.D. Skoromnik

Phys.Rev.A 82, 052703 (2010)

Relativistic case

Relativistic case is of interest for some applications:

- collisions between opposing charge particle beams;**
- analysis of the polarization effects.**

QFT model

$$H = \frac{\vec{p}^2}{2} + \sum_{\vec{k}} \omega_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} + \frac{g}{\sqrt{2\Omega}} \sum_{\vec{k}} A_{\vec{k}} \left(e^{i\vec{k}\cdot\vec{r}} a_{\vec{k}} + e^{-i\vec{k}\cdot\vec{r}} a_{\vec{k}}^\dagger \right)$$

Our model

$$A_{\vec{k}} = \frac{1}{\sqrt{k}}$$

Polaron model

$$A_{\vec{k}} = \frac{1}{k}$$
$$\omega_{\vec{k}} = 1$$

$$\vec{P} = \vec{p} + \sum_{\vec{k}} \vec{k} a_{\vec{k}}^\dagger a_{\vec{k}}$$

Total momentum

$$[H, \vec{P}] = 0$$

Perturbation theory (1)

$$H = \overbrace{\frac{(\vec{P} - \sum_{\vec{k}} \vec{k} a_{\vec{k}}^\dagger a_{\vec{k}})^2}{2}}^{H_0} + \sum_{\vec{k}} \omega_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}} + \underbrace{\frac{g}{\sqrt{2\Omega}} \sum_{\vec{k}} A_{\vec{k}} (e^{i\vec{k}\cdot\vec{r}} a_{\vec{k}} + e^{-i\vec{k}\cdot\vec{r}} a_{\vec{k}}^\dagger)}_V}$$

$$E_0^{(2)} = \epsilon_0 - \sum_{m \neq 0} \frac{|V_{m0}|^2}{\epsilon_m - \epsilon_0}$$

$$|\psi_{\vec{P},0}^{(0)}\rangle = \frac{e^{i\vec{P}\cdot\vec{r}}}{\sqrt{\Omega}} |0\rangle \longrightarrow \epsilon_0 = \frac{P^2}{2}$$

$$|\psi_{\vec{P}_1,1_{\vec{k}}}^{(0)}\rangle = \frac{e^{i(\vec{P}_1 - \vec{k})\cdot\vec{r}}}{\sqrt{\Omega}} |1_{\vec{k}}\rangle \longrightarrow \epsilon_m = \frac{P_1^2}{2} + \frac{k^2}{2} - \vec{P}_1 \cdot \vec{k} + k$$

$$\langle \psi_{\vec{P},0}^{(0)} | V | \psi_{\vec{P}_1,1_{\vec{k}}}^{(0)} \rangle = \frac{g}{\sqrt{2\Omega}} A_{\vec{k}} \frac{(2\pi)^3 \delta(\vec{P}_1 - \vec{P})}{\Omega}$$

Perturbation theory (2)

$$E^{(2)} = \frac{P^2}{2} - \frac{g^2}{16\pi^3} \int \frac{d\vec{k}}{k[k^2/2 - \vec{P} \cdot \vec{k} + k]}$$

$$E^{(2)} \approx E_b + \frac{P^2}{2m^*}$$

$$E_b = -\frac{g^2}{2\pi^2} \ln \left(\frac{K}{2} + 1 \right)$$

$$E_b^{\text{polaron}} \simeq -\frac{g^2}{8\pi}$$

$$\equiv -\frac{g^2}{16\pi^3} \int \frac{d\vec{k}}{k[k^2/2 + k]}$$

$$+ \underbrace{\frac{P^2}{2} - \frac{g^2}{16\pi^3} \int \frac{d\vec{k}}{k[k^2/2 + k]^3} (\vec{P} \cdot \vec{k})^2}_{\text{mass correction}}$$

$$m^* \simeq 1 + \frac{g^2}{6\pi^2}$$

OM for QFT model

First step is the choice of the basis taking into account the qualitative peculiarities of the system

1. Selection of the classical component of the field from creation and annihilation operators.
2. The possibility to create a localized state in this classical field
In analogy with polaron problem
3. The variational state vectors should be eigenstates of the total momentum operator of the system.

$$|\Psi(\vec{r}, \vec{R})\rangle = \phi(\vec{r} - \vec{R}) \exp \left(\sum_{\vec{k}} \left(u_{\vec{k}}^* e^{-i\vec{k} \cdot \vec{R}} a_{\vec{k}}^\dagger - \frac{1}{2} |u_{\vec{k}}|^2 \right) \right) |0\rangle$$

$\phi(\vec{r} - \vec{R})$ particle wave function

\vec{R} localization point in space

$u_{\vec{k}}$ classical component of the field

Choice of the trial state vector (1)

$$\frac{\delta}{\delta u_{\vec{k}}} \left[\langle \Psi(\vec{r}, \vec{R}) | \mathbf{H} | \Psi(\vec{r}, \vec{R}) \rangle \right] = \frac{\delta}{\delta \phi(\vec{r} - \vec{R})} \left[\langle \Psi(\vec{r}, \vec{R}) | \mathbf{H} | \Psi(\vec{r}, \vec{R}) \rangle \right] = 0$$

$$u_{\vec{k}} = - \frac{g}{\sqrt{2\Omega\omega_{\vec{k}}^3}} \int d\vec{r} |\phi(\vec{r})|^2 e^{-i\vec{k}\cdot\vec{r}}$$

$$\phi(\vec{r}) = \frac{\lambda^{\frac{3}{2}}}{\pi^{\frac{3}{4}}} e^{-\frac{\lambda^2 r^2}{2}}$$

Choice of the trial state vector (2)

The introduced wave functions satisfy two conditions, however, they are not translationally invariant. Moreover, they are degenerate. The choice of the correct linear combination of these wave functions leads to the eigenstates of the total momentum of the system

$$|\Psi_{\vec{P}_1, n_{\vec{k}}}^{(0)}\rangle = \frac{1}{N_{\vec{P}_1, n_{\vec{k}}} \sqrt{\Omega}} \int d\vec{R} \phi_{\vec{P}_1}(\vec{r} - \vec{R}) \exp\left\{i(\vec{P}_1 - \vec{k}n_k) \cdot \vec{R}\right\} \exp\left\{\sum_{\vec{k}} (u_k e^{-i\vec{k}\vec{R}} \mathbf{a}_k^\dagger - u_k^* e^{i\vec{k}\vec{R}} \mathbf{a}_k)\right\} |n_{\vec{k}}\rangle$$

Zero order approximation

$$E_0^{(L)} = \langle \Psi_{\vec{P}}^{(L)} | \mathbf{H} | \Psi_{\vec{P}}^{(L)} \rangle$$

$$|\Psi_{\vec{P}}^{(L)}\rangle = \frac{1}{N_{\vec{P}}\sqrt{\Omega}} \int d\vec{R} \phi_{\vec{P}}(\vec{r} - \vec{R}) \exp(i\vec{P}\vec{R} + \sum_{\vec{k}} (u_{\vec{k}} a_{\vec{k}}^{\dagger} e^{-i\vec{k}\vec{R}} - \frac{1}{2} u_{\vec{k}}^2)) |0\rangle$$

$$E_L^{(0)}(\vec{P}, g) = \frac{P^2}{2} - \vec{P} \cdot \vec{Q} + G + E_f(\vec{P}) + E_{\text{int}}(\vec{P})$$

$$\vec{Q} = \frac{1}{|N_{\vec{P}}|^2} \sum_{\vec{k}} \vec{k} |u_{\vec{k}}|^2 \int d\vec{R} d\vec{r} \phi_{\vec{P}}^*(\vec{r}) \phi_{\vec{P}}(\vec{r} - \vec{R}) e^{\Phi(\vec{R}) + i(\vec{P} - \vec{k}) \cdot \vec{R}}$$

$$E_f(\vec{P}) = \frac{1}{|N_{\vec{P}}|^2} \sum_{\vec{k}} \left(k + \frac{k^2}{2} \right) |u_{\vec{k}}|^2 \int d\vec{R} d\vec{r} \phi_{\vec{P}}^*(\vec{r}) \phi_{\vec{P}}(\vec{r} - \vec{R}) e^{\Phi(\vec{R}) + i(\vec{P} - \vec{k}) \cdot \vec{R}}$$

$$E_{\text{int}}(\vec{P}) = \frac{g}{|N_{\vec{P}}|^2} \sum_{\vec{k}} \frac{u_{\vec{k}}}{\sqrt{2k\Omega}} \int d\vec{R} d\vec{r} \left(\phi_{\vec{P}}^*(\vec{r} + \vec{R}) \phi_{\vec{P}}(\vec{r}) + \phi_{\vec{P}}^*(\vec{r}) \phi_{\vec{P}}(\vec{r} - \vec{R}) \right) e^{\Phi(\vec{R}) + i(\vec{P} \cdot \vec{R} + \vec{k} \cdot \vec{r})}$$

$$\Phi(\vec{R}) = \sum_{\vec{m}} |u_{\vec{m}}|^2 \left(e^{-i\vec{m} \cdot \vec{R}} - 1 \right) \sim g^2$$

Weak coupling limit (1)

$$E_L^{(0)}(0, g) = \sum_{\vec{k}} \left(k + \frac{k^2}{2} \right) |u_{\vec{k}}|^2 \frac{\phi_{\vec{k}}^2}{\phi_0^2} + \frac{2g}{\sqrt{2\Omega}} \sum_{\vec{k}} \frac{u_{\vec{k}}}{\sqrt{k}} \frac{\phi_{\vec{k}}}{\phi_0}$$



$$E_L^{(0)}(0, g) = -g^2 \frac{(-4 + \sqrt{2})^2}{32\pi} \quad \lambda = \frac{\sqrt{3\pi}}{2} (4 - \sqrt{2})$$

Moving particle

$$E_L^{(0)}(P, g) \approx E_L^{(0)}(0, g) + \frac{P^2}{2} \left[1 - \frac{g^2}{9\pi^2} \frac{17 - \sqrt{2}}{21} \right]$$

$$m^{(0)*} = 1 + \frac{g^2}{9\pi^2} \frac{17 - \sqrt{2}}{21}$$

very close to
perturbation-
theory result

$$m^* \simeq 1 + \frac{g^2}{6\pi^2}$$

Weak coupling limit (2)

We see that already in the zero-order approximation the energy of the system is finite and well defined. However, the second iteration for the energy of the system gives a contribution of the same order of magnitude and should be included.

This corresponds to single-phonon intermediate transitions

Second order iteration (1)

$$E_{\mu}^{(2)} = E_{\mu}^{(0)} + \sum_{\nu \neq \mu} \frac{|H_{\mu\nu}|^2}{E_{\mu}^{(0)} - H_{\nu\nu}}$$

H is the **full** Hamiltonian

We break the summation region into two parts

$$H_{\nu\nu} - E_{\mu}^{(0)} = \underbrace{\frac{k^2}{2} + k}_{\text{leading term } \vec{k} < \vec{k}_0} + \underbrace{g^2 I_{\vec{k}}}_{\text{leading term } \vec{k} > \vec{k}_0} - E_0^{(L)}$$



$$\ln \frac{(\frac{k_0^2}{2} + k_0)k_0}{a} = -2|\ln g| + \frac{2}{3} \frac{k_0^2}{\lambda^2}$$

Second order iteration (2)

$$E_L^{(2)} \approx E_0^{(L)} + \sum_{\vec{k} < \vec{k}_0} \frac{-\left(u_{\vec{k}} \frac{\phi_{\vec{k}}}{\phi_0} \left(\frac{k^2}{2} + k\right) + \frac{g}{\sqrt{2\Omega}} \frac{1}{\sqrt{k}}\right)^2}{\left(\frac{k^2}{2} + k\right)} + \sum_{\vec{k} > \vec{k}_0} \frac{\left(-\frac{g}{\sqrt{2\Omega}} \frac{\phi_{\vec{k}} \phi_0}{\sqrt{k}}\right) (-E_0 u_{\vec{k}})}{\phi_{\vec{k}}^2 g^2 I_{\vec{k}}}$$



$$\vec{k} < \vec{k}_0$$

$$E_L^{(2)} \approx E_L^{(0)} - \left[\frac{g^2 \lambda}{24\pi^2} \left(\sqrt{6\pi} \operatorname{Erf} \left(\frac{\sqrt{\frac{3}{2}} k_0}{\lambda} \right) + \lambda - \lambda e^{-\frac{3k_0^2}{2\lambda^2}} \right) - \frac{g^2 \lambda}{2\sqrt{3}\pi^{3/2}} \operatorname{Erf} \left(\frac{\sqrt{3} k_0}{2\lambda} \right) \right]$$

$$- \frac{g^2}{2\pi^2} \ln \left(\frac{k_0}{2} + 1 \right)$$

$$+ E_L^{(0)} \frac{12\sqrt{6\pi}}{5\lambda\pi} e^{-\frac{5k_0^2}{12\lambda^2}}$$

$$\vec{k} > \vec{k}_0$$

Does it remind the result from
perturbation theory?

Second order iteration (3)

$$\lim_{g \rightarrow 0} E^{(2)}(0, g)$$



$$E^{(2)}(0, g) \xrightarrow{g \rightarrow 0} -\frac{g^2}{2\pi^2} \ln \left(\frac{k_0}{2} + 1 \right)$$

$$k_0 \approx \lambda \sqrt{3 |\ln g|}$$

Perturbation theory formula with a well defined cut-off

The energy is a **non-analytical** function of a coupling constant

Second order iteration (4)

$$E^{(2)}(\vec{P}, g) = E^{(2)}(0, g) + \frac{P^2}{2} - \frac{g^2}{2\Omega} \sum_{\vec{k} < \vec{k}_0} \frac{(\vec{P} \cdot \vec{k})^2}{k(k^2/2 + k)^3}$$



$$m^{(2)*} \approx 1 + \frac{g^2}{6\pi^2}$$

The second order iteration for the mass coincides with perturbation theory result

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Regularization of ultraviolet divergence for a particle interacting with a scalar quantum field

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THANK YOU FOR THE ATTENTION !!!

