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The Influence Functional approach to the quantum systems dynamics

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The paper structure

1. Model QS+EMF
2. Density matrix of QS+EMF as a paths integral
3. EMF influence functional
4. Quantum transition probability
   as a paths integral of real functional
5. Some applications

The studied model

$$\hat{H}_{full} = \hat{H}_{sys} + \hat{H}_{field} + \hat{H}_{int}$$

Quantum system: $\hat{H}_{sys}|n\rangle = E_n|n\rangle$

Quantum electromagnetic field:

$$\hat{H}_{field} = \int \frac{d^3k}{(2\pi)^3}\, \hbar\Omega_{\mathbf{k}}(\hat{a}^+_{\mathbf{k}}\hat{a}_{\mathbf{k}} + 1/2),$$

Interaction:

$$\hat{H}_{int} = \int \frac{d^3k}{(2\pi)^3} e\hat{j}^{\mu}(\varepsilon^{\lambda}_{\mu}(\mathbf{k})\hat{a}^+_{\mathbf{k}} + \varepsilon^{\lambda *}_{\mu}(\mathbf{k})\hat{a}_{\mathbf{k}})$$

where $\varepsilon^{\lambda}_{\mu}(\mathbf{k}) = \frac{1}{\sqrt{\Omega_{\mathbf{k}}}} e^{(\lambda)}_{\mu} e^{\imath \mathbf{kx}}$

The system evolution

$$\hat{\rho}_{full}(t) = \hat{U}(t,0)\hat{\rho}_{full}(0)\hat{U}^{+}(t,0)$$

where

$$\hat{U}(t,0) = \hat{T}exp\{-\frac{\imath}{\hbar}\int_0^t \hat{H}_{full}dt'\}$$

The mixed representation

Basis vectors are given in the form $|x, a_{\mathbf{k}}^{\lambda}\rangle = |x\rangle \otimes |a_{\mathbf{k}}^{\lambda}\rangle$

Holomorphic representation properties: $\hat{a}_{\mathbf{k}}^{\lambda}|a_{\mathbf{k}}^{\lambda}\rangle = a_{\mathbf{k}}^{\lambda}|a_{\mathbf{k}}^{\lambda}\rangle$

$$\langle a_{\mathbf{k}}^{\prime\lambda}|a_{\mathbf{k}}^{\lambda}\rangle = \exp\{-\frac{1}{2}(|a_{\mathbf{k}}^{\prime\lambda}|^2 + |a_{\mathbf{k}}^{\lambda}|^2 - 2a_{\mathbf{k}}^{\prime\lambda *}a_{\mathbf{k}}^{\lambda})\}$$

$$1 = \int |a_{\mathbf{k}}^{\lambda}\rangle\langle a_{\mathbf{k}}^{\lambda}| \frac{|a_{\mathbf{k}}^{\lambda}|d|a_{\mathbf{k}}^{\lambda}d\phi_{\mathbf{k}}^{\lambda}}{\pi}$$

where $a_{\mathbf{k}}^{\lambda}$ - complex variable

Coordinate representation properties: $\hat{x}|x\rangle = x|x\rangle$

$$\langle x'|x\rangle = \delta(x' - x)$$

$$1 = \int |x\rangle\langle x|dx$$

The density matrix

$$\rho(a_f^*, x_f, a'_f, x'_f; t) = \int \frac{da_{in}^* a_{in}}{2\pi\imath} \frac{da_{in}'^* a'_{in}}{2\pi\imath} dx_{in} dx'_{in} \times$$

$$\times U(a_f^*, x_f, a_{in}, x_{in}; t) \rho(a_{in}^*, x_{in}, a'_{in}, x'_{in}; 0) U^*(a'_f, x'_f, a_{in}^*, x'_{in}; t)$$

where

$$\rho(a_f^*, x_f, a'_f, x'_f; t) = < a_f, x_f | \hat{\rho}(t) | a'_f, x'_f >$$

$$U(a_f^*, x_f, a_{in}, x_{in}; t) = < a_f, x_f | \hat{U}(t, 0) | a_{in}, x_{in} >$$

The kernel of the evolution operator as a paths integral

$$U(a_f^*, x_f, a_{in}, x_{in}; t) = \int (\prod_{k,\lambda} \mathfrak{D}a_{\mathbf{k}}^{\lambda *} \mathfrak{D}a_{\mathbf{k}}^{\lambda} \mathfrak{D}p \mathfrak{D}x) \times$$

$$\times A \ \exp\{\imath \int_0^t [p\dot{x} - H_{sys}(p,x) + \int \sum_{\lambda} (\frac{\dot{a}_{\mathbf{k}}^{\lambda *} a_{\mathbf{k}}^{\lambda} - a_{\mathbf{k}}^{\lambda *} \dot{a}_{\mathbf{k}}^{\lambda}}{2\imath} - H_{field}(a_{\mathbf{k}}^{\lambda *}, a_{\mathbf{k}}^{\lambda})) \frac{d^3k}{(2\pi)^3} -$$

$$- \int \frac{d^3k}{(2\pi)^3} \sum_{\lambda} j^{\mu}(x)(\varepsilon_{\mu}^{\lambda}(\mathbf{k}) a_{\mathbf{k}}^{\lambda *} + \varepsilon_{\mu}^{\lambda *}(\mathbf{k}) a_{\mathbf{k}}^{\lambda})] dt' \}$$

Additional functional A represents the boundary conditions

$$A = exp\{\frac{1}{2}(\int \sum_{\lambda} (a_{\mathbf{k}}^{\lambda *}(t) a_{\mathbf{k}}^{\lambda}(t) + a_{\mathbf{k}}^{\lambda *}(0) a_{\mathbf{k}}^{\lambda}(0)) \frac{d^3k}{(2\pi)^3})\}$$

Fadeev L. D., Slavnov A. A. Gauge Fields. Introduction to Quantum theory // Addison-Wesley P. C., 1991.

Feynman R. P., Hibbs A. R. Quantum mechanics and Path Integrals // N.Y.: McGraw-Hill, 1965

The density matrix as a paths integral

$$\rho(a_f^*, x_f, a'_f, x'_f; t) = \int (\prod_{k,k',\lambda,\lambda'} \mathfrak{D}a_{\mathbf{k}}^{\lambda *} \mathfrak{D}a_{\mathbf{k}}^{\lambda} \mathfrak{D}p \mathfrak{D}x \mathfrak{D}a_{\mathbf{k}}'^{\lambda *} \mathfrak{D}a_{\mathbf{k}}'^{\lambda} \mathfrak{D}p' \mathfrak{D}x') \frac{da_{in}^* a_{in}}{2\pi\imath} \frac{da_{in}'^* a'_{in}}{2\pi\imath} dx_{in} dx'_{in} \times$$

$$\times A \ \exp\{\imath \int_0^t [p\dot{x} - H_{sys}(p,x) + \int \sum_{\lambda} (\frac{\dot{a}_{\mathbf{k}}^{\lambda *} a_{\mathbf{k}}^{\lambda} - a_{\mathbf{k}}^{\lambda *} \dot{a}_{\mathbf{k}}^{\lambda}}{2\imath} - H_{field}(a_{\mathbf{k}}^{\lambda *}, a_{\mathbf{k}}^{\lambda})) \frac{d^3k}{(2\pi)^3} -$$

$$- \int \frac{d^3k}{(2\pi)^3} \sum_{\lambda} j^{\mu}(x) (\varepsilon_{\mu}^{\lambda}(\mathbf{k}) a_{\mathbf{k}}^{\lambda *} + \varepsilon_{\mu}^{\lambda *}(\mathbf{k}) a_{\mathbf{k}}^{\lambda})] dt' \} \rho(a_{in}^*, x_{in}, a'_{in}, x'_{in}; 0) \times$$

$$\times A' \ \exp\{\imath \int_0^t [p'\dot{x'} - H_{sys}(p',x') + \int \sum_{\lambda'} (\frac{\dot{a'}_{\mathbf{k'}}^{\lambda' *} a_{\mathbf{k'}}^{\prime \lambda'} - a_{\mathbf{k'}}^{\lambda' *} \dot{a'}_{\mathbf{k'}}^{\lambda'}}{2\imath} - H_{field}(a_{\mathbf{k'}}^{\prime \lambda' *}, a_{\mathbf{k'}}^{\prime \lambda'})) \frac{d^3k'}{(2\pi)^3} -$$

$$- \int \frac{d^3k'}{(2\pi)^3} \sum_{\lambda'} j^{\mu}(x') (\varepsilon_{\mu}^{\lambda'}(\mathbf{k'}) a_{\mathbf{k'}}^{\prime \lambda' *} + \varepsilon_{\mu}^{\lambda' *}(\mathbf{k'}) a_{\mathbf{k'}}^{\prime \lambda'})] dt' \}$$

The density matrix for quantum system

$$\rho_{sys}(x_f, x'_f) - ?$$

At initial moment $t = 0$:

$$\rho(a^*_{in}, x_{in}, a'_{in}, x'_{in}; 0) = \rho_{sys}(x_{in}, x'_{in}; 0) \cdot \rho_{field}(a^*_{in}, a'_{in}; 0)$$

Reduction of the total density matrix to the density matrix investigated system

$$\rho_{sys}(x_f, x'_f; t) = Sp_{a'_f = a_f} \rho(a^*_f, x_f, a'_f, x'_f; t)$$

The influence functional definition

The equation of this density matrix evolution can be written as

$$\rho_{sys}(x_f, x'_f; t) = \int \mathfrak{D}p\mathfrak{D}x\mathfrak{D}p'\mathfrak{D}x' dx_{in} dx'_{in} \times$$

$$\times \exp\{-\frac{\imath}{\hbar} S_{sys}\} F_{field}[x, x'] \rho_{sys}(x_{in}, x'_{in}; 0) \exp\{\frac{\imath}{\hbar} S'^{*}_{sys}\},$$

$F[x, x']$ – functional describing electromagnetic field influence on investigated quantum system

where investigated system action is

$$S_{sys} = \int_0^t [p(t')\dot{x}(t') - H_{sys}(p(t'), x(t'))] dt'$$

The influence functional definition

$$F_{field}[x,x'] = Sp_{a_f=a'_f}\int(\prod_{k,k',\lambda,\lambda'}\mathfrak{D}a_{\mathbf{k}}^{\lambda *}\mathfrak{D}a_{\mathbf{k}}^{\lambda}\mathfrak{D}a_{\mathbf{k}'}^{\prime\lambda',*}\mathfrak{D}a_{\mathbf{k}'}^{\prime\lambda'})\frac{da_{in}^{*}a_{in}}{2\pi\imath}\frac{da_{in}^{\prime *}a'_{in}}{2\pi\imath}\times$$

$$\times\ A\exp\{-\frac{\imath}{\hbar}S_{infl}\}\rho_{field}(a_{in}^{*},a'_{in};0)A'^{*}\exp\{\frac{\imath}{\hbar}S'_{infl}\}$$

where action, describes influence electromagnetic field on investigated system is

$$S_{infl} = \int_0^t[\int\sum_{\lambda}(\frac{\dot{a}_{\mathbf{k}}^{\lambda *}a_{\mathbf{k}}^{\lambda}-a_{\mathbf{k}}^{\lambda *}\dot{a}_{\mathbf{k}}^{\lambda}}{2\imath}-H_{field}(a_{\mathbf{k}}^{\lambda *},a_{\mathbf{k}}^{\lambda}))\frac{d^3k}{(2\pi)^3}-$$

$$-\int\frac{d^3k}{(2\pi)^3}\sum_{\lambda}j^{\mu}(x)(\varepsilon_{\mu}^{\lambda}(\mathbf{k})a_{\mathbf{k}}^{\lambda *}+\varepsilon_{\mu}^{\lambda *}(\mathbf{k})a_{\mathbf{k}}^{\lambda})]dt'$$

The Influence Functional calculation

In general, the influence functional explicit form depends on

a) EMF initial and finite states
b) Model of EMF and investigated system interaction

In 1963 R. Feynman introduced the influence functional and studied some of its properties.

We have done influence functional calculations for different models in holomorphic space of EMF paths.

Feynman R. P., Vernon F. L. The Theory of a General Quantum System Interacting with a Linear Dissipative System // Annals of Physics, 1963, 24, Issue 1, p.118-173

Feynman R. P., Hibbs A. R. Quantum mechanics and Path Integrals // N.Y.: McGraw-Hill, 1965

Vacuum electromagnetic field influence functional

$$F^{vac\to vac}[x,x'] = \exp\{-\int_0^t \int_0^{t'} [\gamma(t',t'')j(x(t'))j(x(t'')) + \gamma^*(t',t'')j(x'(t'))j(x'(t''))]\}dt''dt'\}$$

$$F^{vac}[x,x'] = F^{vac\to vac}[x,x'] \cdot$$

$$\cdot \exp\{\int_0^t \int_0^{t'} [\gamma^*(t',t'')j(x(t'))j(x'(t'')) + \gamma(t',t'')j(x'(t'))j(x(t''))]dt''dt'\}$$

where functions $\gamma(t',t'')$ depend on fundamental constant and time moments

$$\gamma(t',t'') = \frac{e^2}{\hbar^2}\frac{\hbar\Omega_k}{2\varepsilon_0 V}e^{-i\Omega_k(t'-t'')}$$

The coherent electromagnetic field influence functional

The initial state of EMF is pure coherent

$$\zeta_\alpha(\alpha_{in}^*) = \langle \alpha_{in} | \alpha \rangle = e^{-\frac{|\alpha_{in}|^2}{2} - \frac{|\alpha|^2}{2}} e^{\alpha_{in}^* \alpha}$$

$$F^{coh}[x, x'] = F^{vac}[x, x'] \cdot$$

$$\cdot \exp\{-\frac{\imath}{\hbar}\sqrt{\frac{\hbar\Omega_k}{2\varepsilon_0 V}} e \int_0^t (j(x'(t')) - j(x(t'))) \cos(\Omega_k t' - \phi_k) dt'\}$$

The mixed coherent electromagnetic field influence functional

$$F_k^{Temp}[x,x'] = F_k^{vac}[x,x']\cdot$$

$$\cdot \exp\{-\frac{q^2}{\hbar^2}\frac{\hbar\Omega_k\langle n\rangle_k}{2\varepsilon_0 V}\int_0^t\int_0^t (j(x(t'))-j(x'(t')))(j(x(t''))-j(x(t')))e^{\imath\Omega_k(t'-t'')}dt'dt''\},$$

where

$$\langle n\rangle_k = [e^{\frac{\hbar\Omega_k}{k_B T}}-1]^{-1}$$

The multimode field influence functional

Influence functional multimode EMF can be obtained by the product of all independent modes influence functionals, following Feynman:

$$F^{Temp}[x,x'] = \prod_k F_k^{Temp}[x,x'] = F^{vac}[x,x'] \cdot$$

$$\cdot \exp\{-\frac{q^2}{\hbar^2}\sum_k \frac{\hbar\Omega_k\langle n\rangle_k}{2\varepsilon_0 V}\int_0^t\int_0^t (j(x(t'))-j(x'(t')))(j(x(t''))-j(x(t')))e^{i\Omega_k(t'-t'')}dt'dt''\}$$

$$F^{vac}[x,x'] = \prod_k F_k^{vac}[x,x']$$

These rules are valid for all considered models.

The influence functional general form

On the basis of the calculated influence functionals its general form can be written so

$$F[x,x'] = \exp[\frac{1}{\hbar}S_{0F}[x,x']]\exp[\frac{i}{\hbar}S_F[x,x']]$$

where $S_{0F}[x,x']$ and $S_F[x,x']$ are real functionals along paths in the investigated system trajectories space.

These functionals lead to different effects of the EMF influence on the target system.

Having used this general form for influence functional the density matrix is to be represented so

$$\rho_{sys}(x_f, x'_f; t) = \int \mathfrak{D}p\mathfrak{D}x\mathfrak{D}p'\mathfrak{D}x' dx_{in} dx'_{in} \times$$

$$\times \exp\{\frac{1}{\hbar} S_{0F}[x, x']\} \exp\{-\frac{i}{\hbar}(S_{sys}[p, x] - S_{sys}[p', x'] - S_F[x, x'])\} \rho_{sys}(x_{in}, x'_{in}; 0)$$

Quantum transition probability

Probability observation of quantum system in state $|m\rangle$ with energy E_m:

$$P(m,t) = \int \phi_m^*(x_f)\rho(x_f, x'_f; t)\phi_m(x'_f)dx_f dx'_f =$$

$$= \int \mathfrak{D}p\mathfrak{D}x\mathfrak{D}p'\mathfrak{D}x' dx_f dx'_f dx_{in} dx'_{in}\ \phi_m^*(x_f)\phi_m(x'_f)\times$$

$$\times \exp\{\frac{1}{\hbar}S_{0F}[x,x']\}\exp\{-\frac{i}{\hbar}(S_{sys}[p,x] - S_{sys}[p',x'] - S_F[x,x'])\}\rho_{sys}(x_{in}, x'_{in}; 0)$$

Quantum transition probability

If initial state is pure quantum state $|n\rangle$ with energy E_n,

then initial density matrix is

$$\rho_{sys}(x_{in}, x'_{in}; 0) = \phi_n^*(x_{in})\phi_n(x'_{in})$$

And probability of quantum transition $|n\rangle$ at initial moment $t = 0$

to $|m\rangle$ at final moment t is

$$P(m, t|n, 0) = \int \mathfrak{D}p\mathfrak{D}x\mathfrak{D}p'\mathfrak{D}x' dx_f dx'_f dx_{in} dx'_{in}\ \phi_m^*(x_f)\phi_m(x'_f)\times$$

$$\times \exp\{\frac{1}{\hbar}S_{0F}[x, x']\} \exp\{-\frac{i}{\hbar}(S_{sys}[p, x] - S_{sys}[p', x'] - S_F[x, x'])\}\phi_n^*(x_{in})\phi_n(x'_{in})$$

Quantum transition probability

Using Euler's formula we express transition probability in the following form

$$P(m,t|n,0) = \int \mathfrak{D}p\mathfrak{D}x\mathfrak{D}p'\mathfrak{D}x' dx_f dx'_f dx_{in} dx'_{in}\ \phi^*_m(x_f)\phi_m(x'_f)\times$$

$$\times \exp\{\frac{1}{\hbar}S_{0F}[x,x']\}\cos\{\frac{1}{\hbar}(S_{sys}[p,x] - S_{sys}[p',x'] - S_F[x,x'])\}\phi^*_n(x_{in})\phi_n(x'_{in}) -$$

$$-\imath \int \mathfrak{D}p\mathfrak{D}x\mathfrak{D}p'\mathfrak{D}x' dx_f dx'_f dx_{in} dx'_{in}\ \phi^*_m(x_f)\phi_m(x'_f)\times$$

$$\times \exp\{\frac{1}{\hbar}S_{0F}[x,x']\}\sin\{\frac{1}{\hbar}(S_{sys}[p,x] - S_{sys}[p',x'] - S_F[x,x'])\}\phi^*_n(x_{in})\phi_n(x'_{in})$$

Quantum transition probability as paths integral of real functional

$$S_{0F}[x,x'] = S_{0F}[x',x] \qquad S_F[x,x'] = -S_F[x',x]$$

$$\phi_m^*(x_f)\phi_m(x'_f) = \phi_m^*(x'_f)\phi_m(x_f) \qquad \phi_n(x_{in})\phi_n^*(x'_{in}) = \phi_n(x'_{in})\phi_n^*(x_{in})$$

If this expressions are valid, then

$$P(m,t|n,0) = \int \mathfrak{D}p\mathfrak{D}x\mathfrak{D}p'\mathfrak{D}x' dx_f dx'_f dx_{in} dx'_{in} \phi_m^*(x_f)\phi_m(x'_f)\times$$

$$\times \exp\{\frac{1}{\hbar}S_{0F}[x,x']\}\cos\{\frac{1}{\hbar}(S_{sys}[p,x] - S_{sys}[p',x'] - S_F[x,x'])\}\phi_n(x_{in})\phi_n^*(x'_{in})$$

Ryazanov G. V. Quantum-mechanical probability as a sum over path // JETP. 1958. V. 35. №1

Model for calculations

For this approach demonstration we are to deal with

1. A QS model is a **particle in one-dimensional infinite potential well**.

2. Initial state of EMF is **a onemode pure coherent state**. We are also considering such processes in which **it is possible to neglect influence vacuum EMF.**

3. Interaction between QS and EMF is chosen by us in the **dipole approximation**.

Quantum transition probability as a paths sum of real functional

The energy representation is more convenient for numerical calculations. Thus we write transition probability in the following form:

$$P(n_f, t_f | n_{in}, t_{in}) = \sum_{n_1,..,n_K=1}^{N} \sum_{m_1,..,m_K=1}^{N} \int_0^1 .. \int_0^1 \times$$

$$\times \cos[S[n_f, n_K, \xi_K; ..; n_k, n_{k-1}, \xi_{k-1}; ..; n_1, n_{in}, \xi_0] -$$

$$-S[n_f, m_K, \zeta_K; ..; m_k, m_{k-1}, \zeta_{k-1}; ..; m_1, n_{in}, \zeta_0]] d\xi_0 .. d\xi_K d\zeta_0 .. d\zeta_K$$

$$S[n_f, n_K, \xi_K; ..; n_k, n_{k-1}, \xi_{k-1}; ..; n_1, n_{in}, \xi_0] = \sum_{k=1}^{K+1} S[n_k, n_{k-1}, \xi_{k-1}]$$

Energy representation

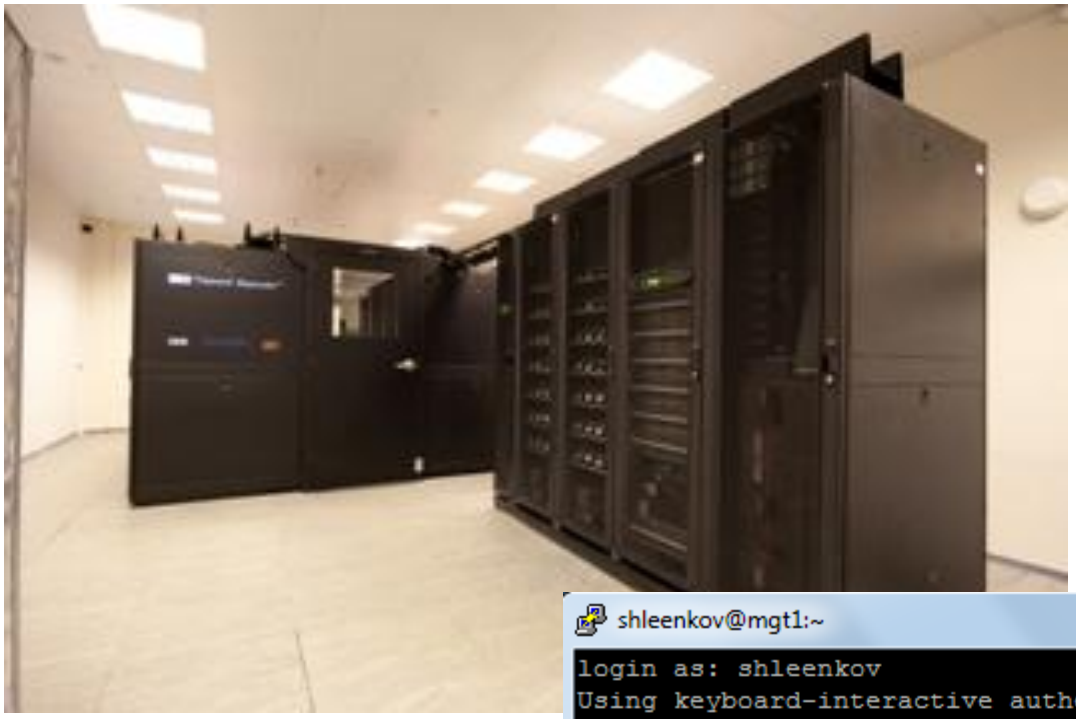
Scully M. O., Zubairy M. S. Quantum Optics // Cambridge University Press. 1997

Here the action in energy representation is

$$S[n_k, t_k; n_{k-1}, t_{k-1}; \xi_{k-1}] = 2\pi(n_k - n_{k-1})\xi_{k-1} + \Omega^R_{n_k n_{k-1}} \times$$

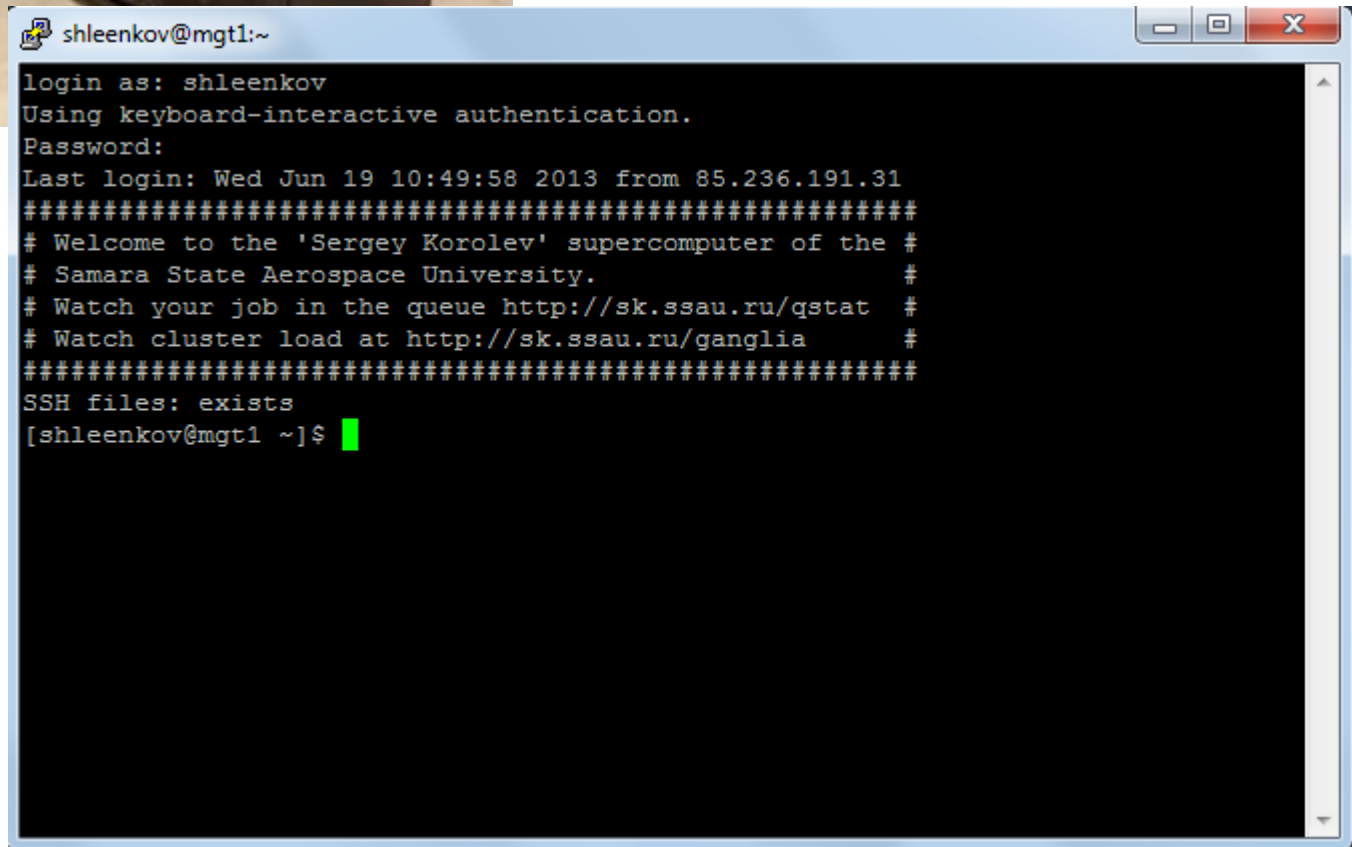
$$\times(\cos(2\pi(n_k - n_{k-1})\xi_{k-1} + (\Omega + \omega_{n_k, n_{k-1}})\frac{t_k + t_{k-1}}{2}) +$$

$$+ \cos(2\pi(n_k - n_{k-1})\xi_{k-1} - (\Omega - \omega_{n_k, n_{k-1}})\frac{t_k + t_{k-1}}{2}))(t_k - t_{k-1}).$$



Supercomputer “Sergey Korolev”

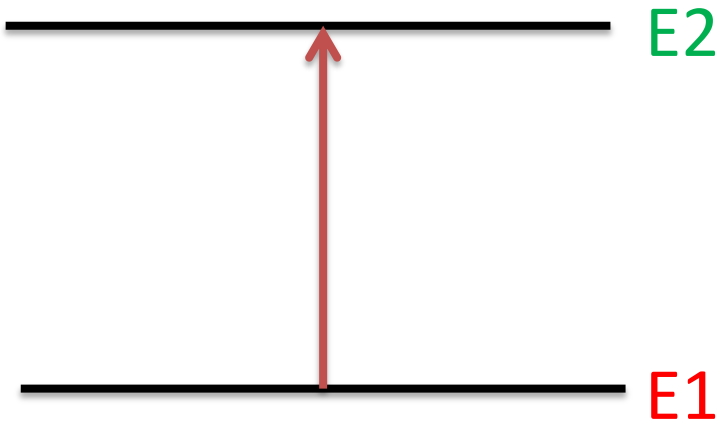
The program was made in C environment



Applications

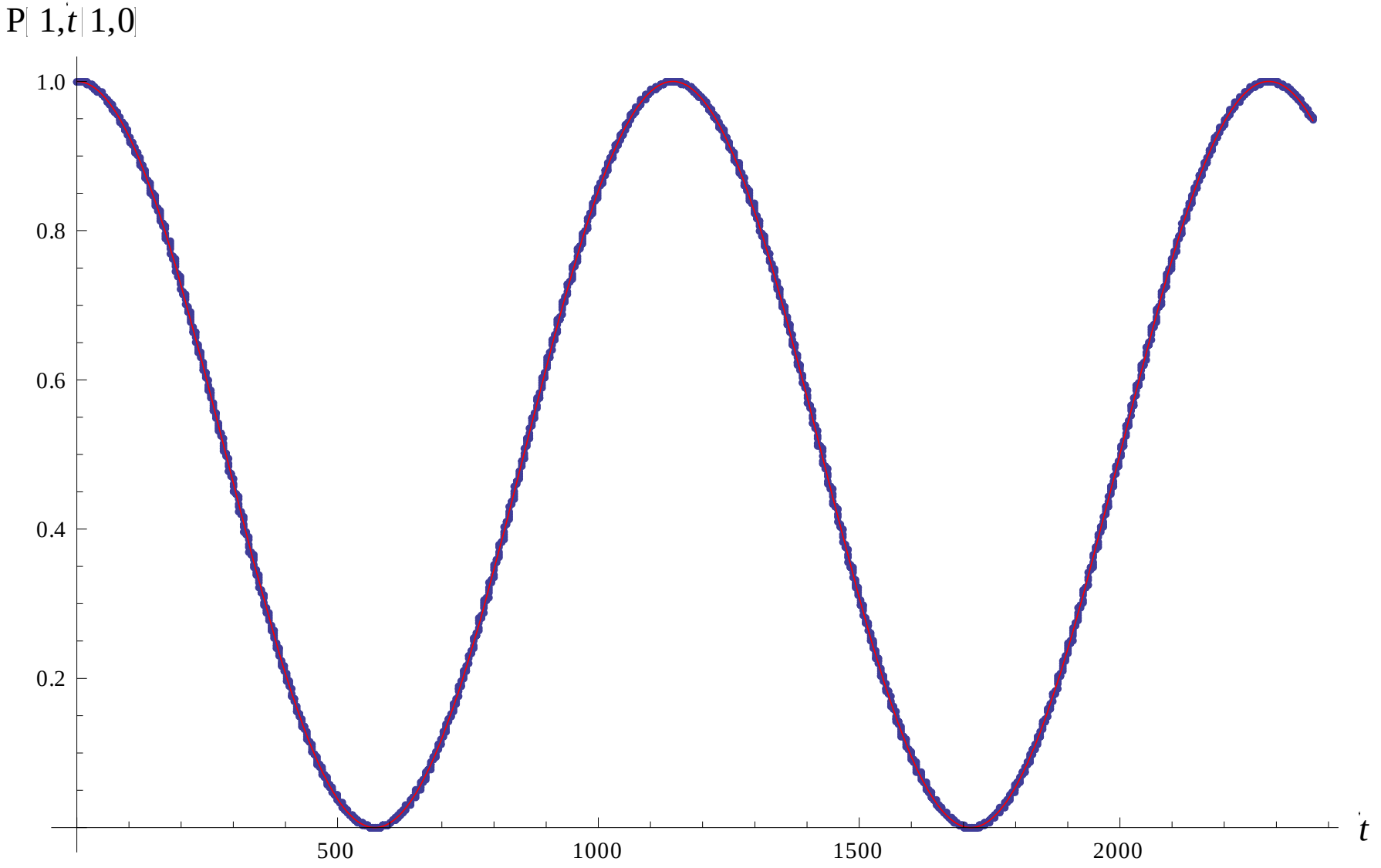
one-photon Rabi oscillation
without RWA

Two-level QS
in the resonance case



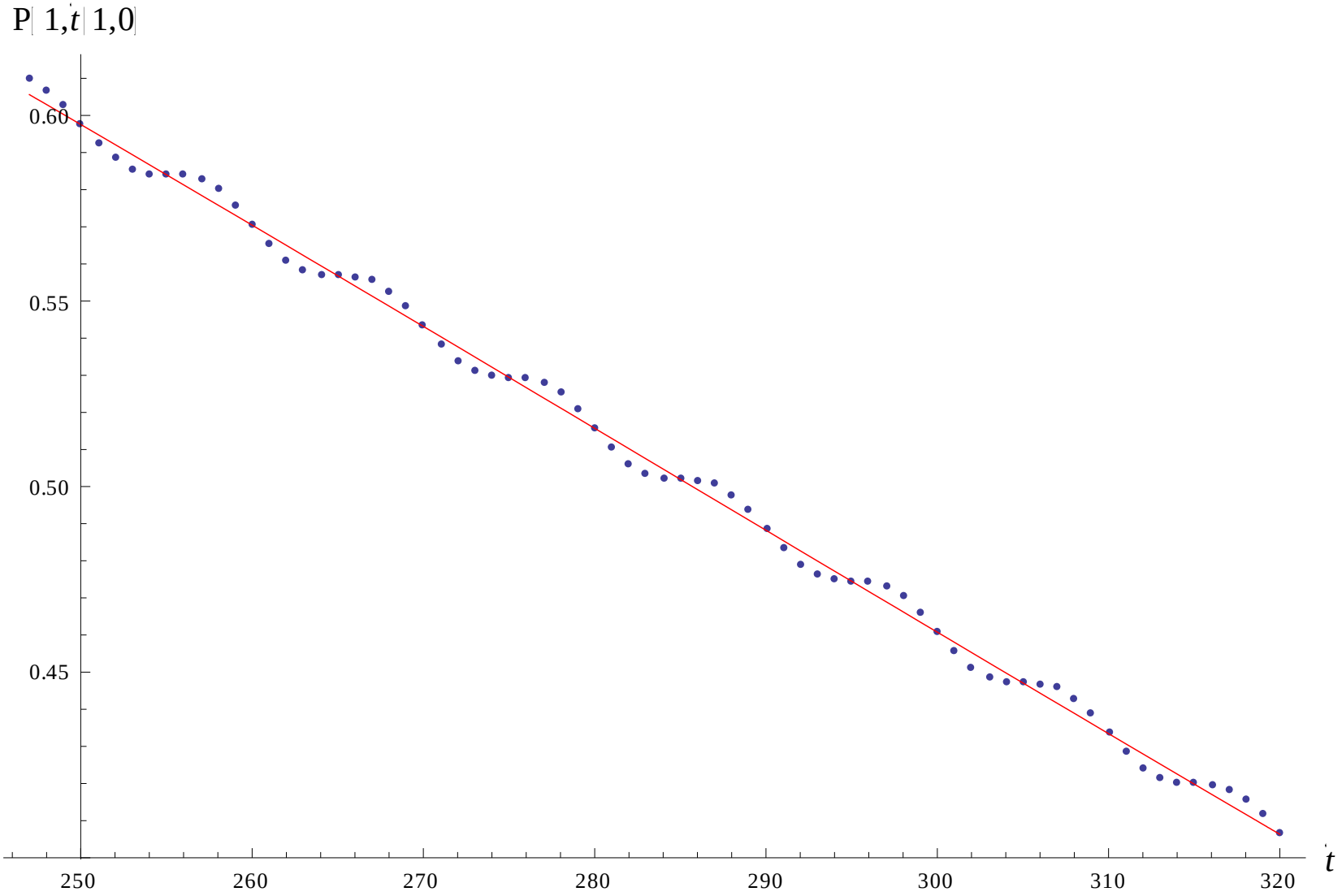
Applications

one-photon Rabi oscillation without RWA



Applications

one-photon Rabi oscillation without RWA

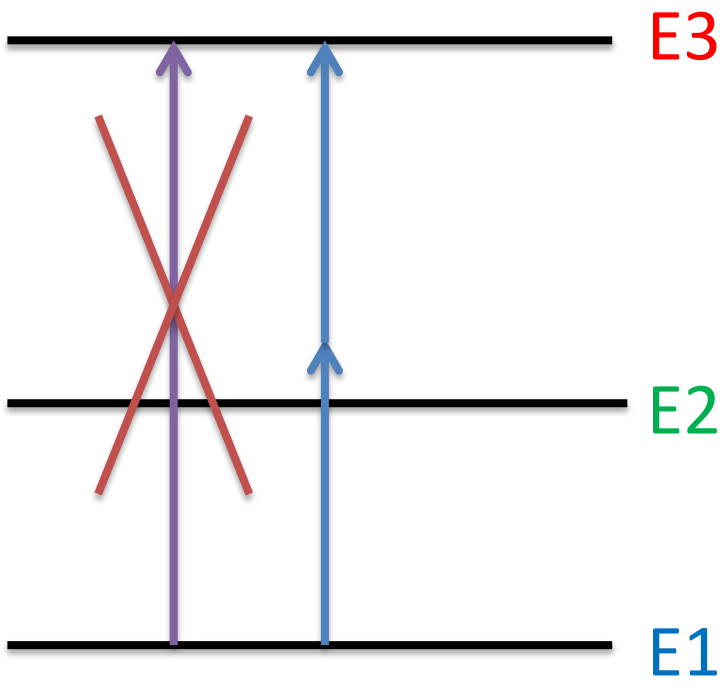


Applications

Multi-photon processes

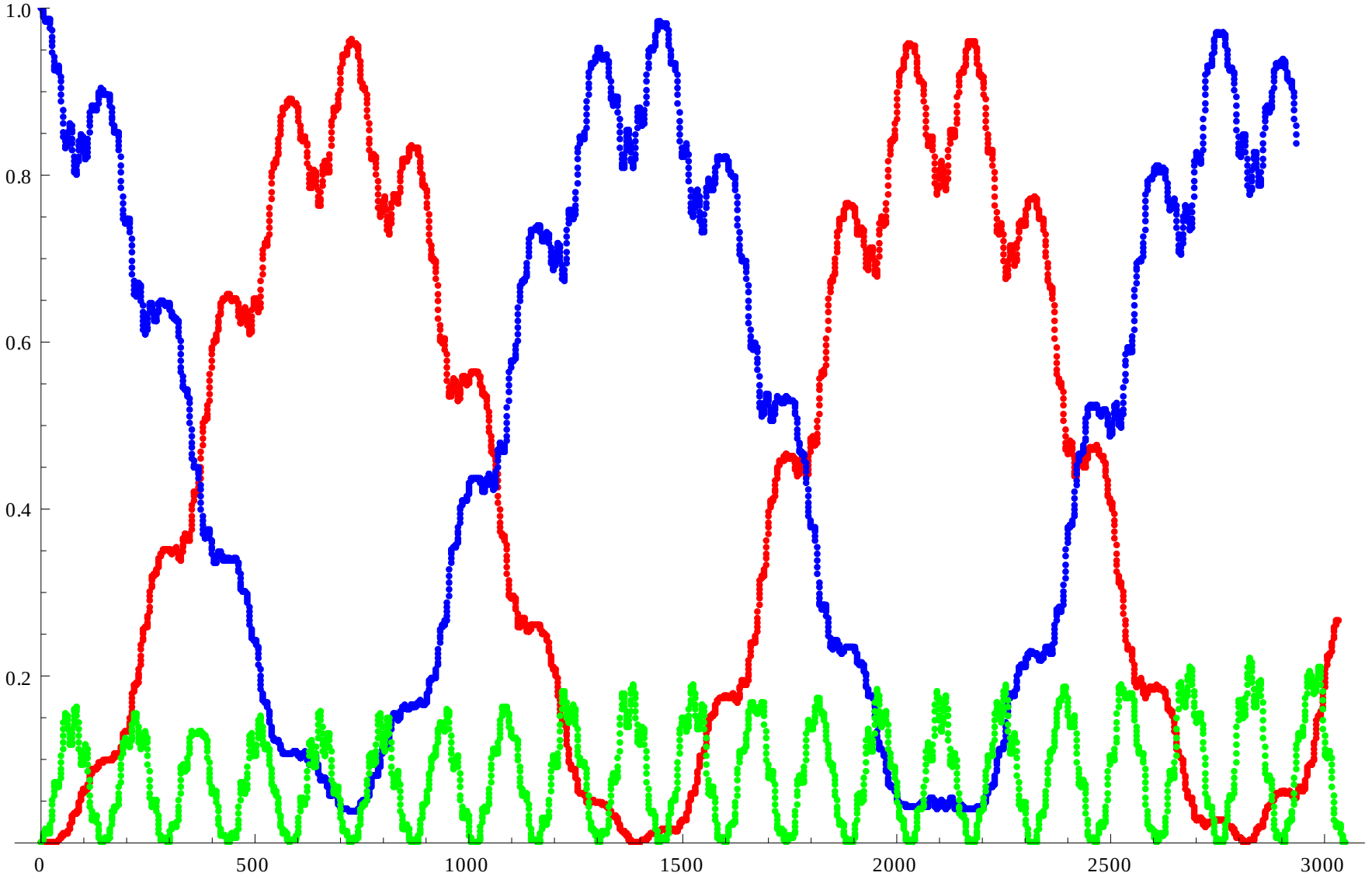
two-photon Rabi oscillation
without RWA

Three-levels QS
Two-photon resonance case



Applications

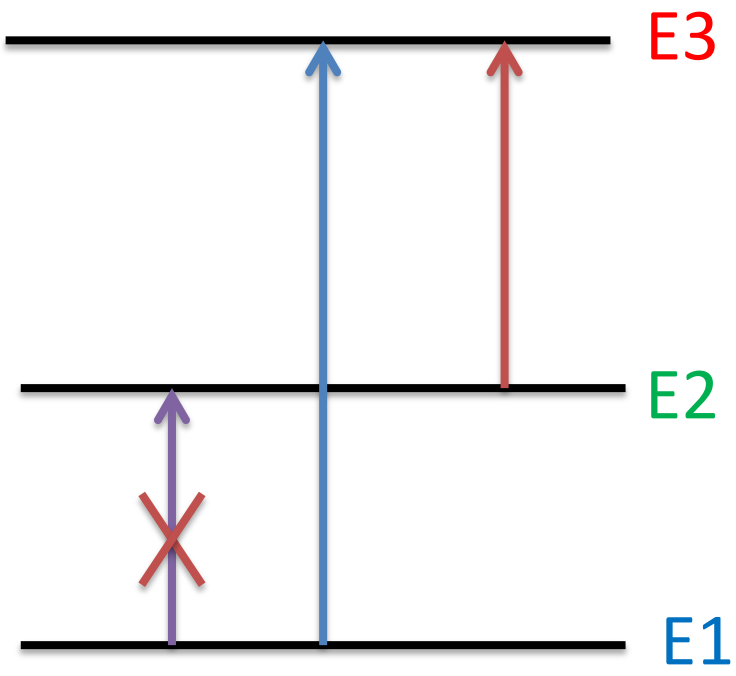
two-photon Rabi oscillation without RWA



Applications

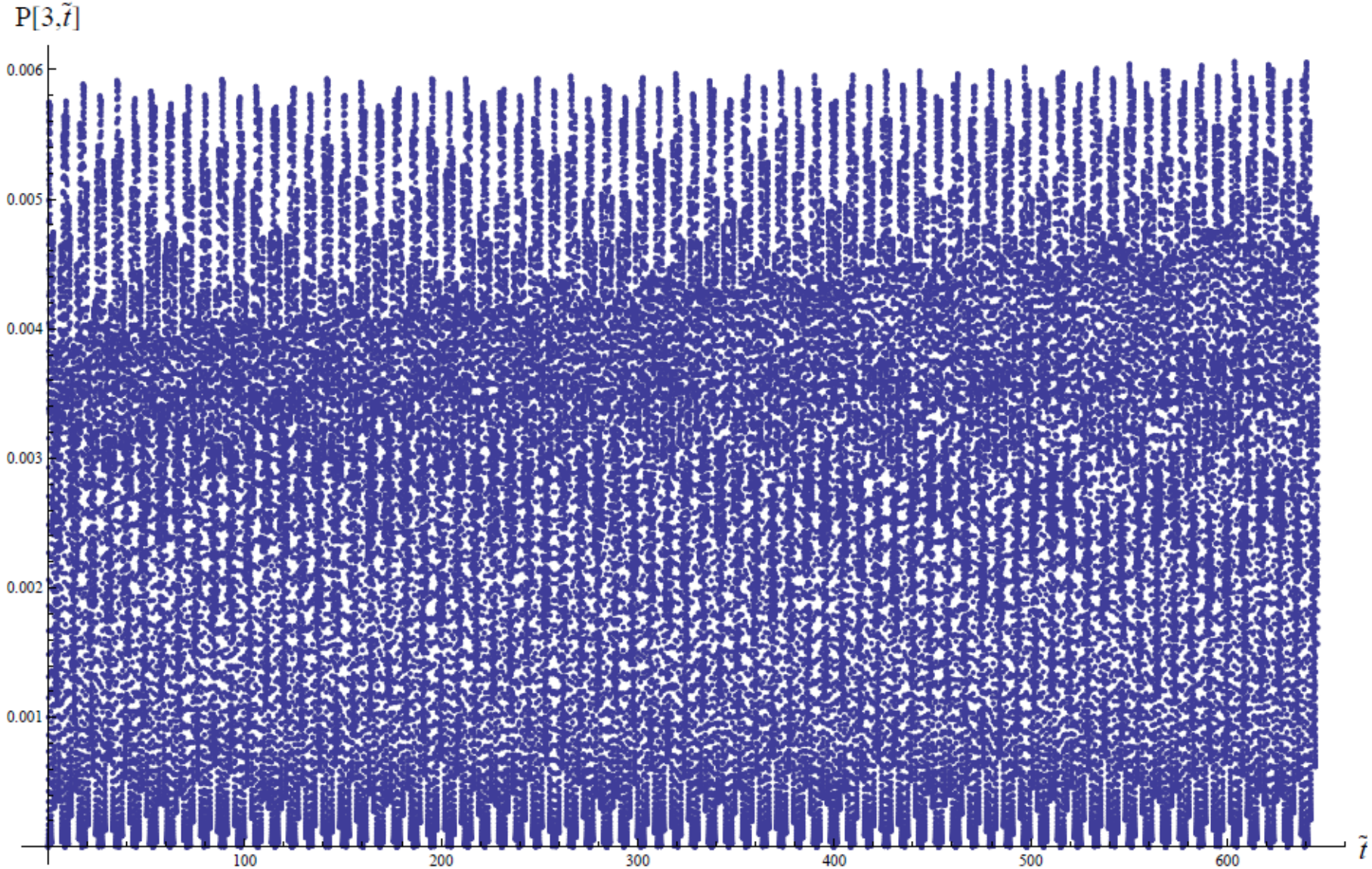
Coherent population trapping

Three-levels QS
Two one-photons resonance cases



Applications

Coherent population trapping



Conclusion

- The Influence Functional approach allows us to describe the investigated quantum system dynamics by integrating of functional along path.

- This functional is sign variable and it is given by the product of exponent and cosine.

- The obtained formula can be used to describe multi-photon processes in many cases.

Thanks for your attention