Sign problems in path integral formulations of quantum mechanics and quantum statistics

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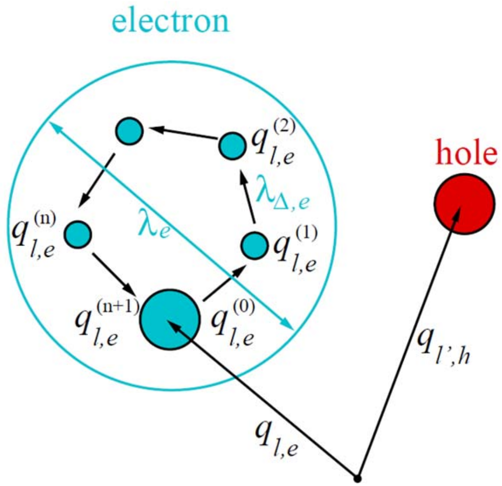
Wiener and Feynman path integrals

$$\hat{H} = \sum_{a=1}^{N} \frac{\hat{p}_a{}^2}{2m_a} + U(\hat{q}_1, \hat{q}_2, \ldots, \hat{q}_N) \quad [\hat{p}_i, \hat{q}_j] = -i\hbar\delta_{ij}$$

$$Z = Tr.[\hat{\rho}] \quad \hat{\rho} = e^{-\beta\left(\hat{K}+\hat{U}\right)} \neq e^{-\beta\hat{K}} \cdot e^{-\beta\hat{U}}$$



1. Operator identity : $e^{-\beta\hat{H}} \equiv e^{-\frac{\beta}{M}\hat{H}} \cdot e^{-\frac{\beta}{M}\hat{H}} \cdot \ldots \cdot e^{-\frac{\beta}{M}\hat{H}}$

2. Operator of unit expansion: $\hat{1} \equiv \int d^{3N}q |q\rangle\langle q|$

3. High temperature approximation:

$$\left\langle q^m \left| e^{-\varepsilon\hat{H}} \right| q^{m+1} \right\rangle \approx \lambda_\varepsilon{}^{-3N} \cdot \exp\left\{ -\frac{\pi}{\lambda_\varepsilon{}^2} \sum_{a=1}^{N} \left(q_a{}^{m+1} - q_a{}^m\right)^2 - \varepsilon U\left(q^m\right) \right\} + O\left((\beta/M)^2\right)$$

$m = 0, \ldots, M-1$ is 'discrete time', λ – thermal wave length

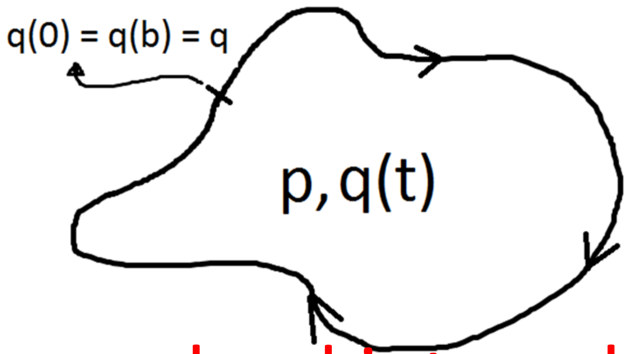
Path integral representation of the Wigner function. Two type of the sign problems.

$$W(p,q) = Z^{-1}\int d^{3N}\xi \exp\left(\frac{i}{\hbar}\langle p|\xi\rangle\right)\cdot\sum_P(-1)^P\left\langle q-\xi/2\left|e^{-\beta\hat{H}}\right|P(q+\xi/2)\right\rangle$$

$$W(p,q) = Z^{-1}\int d^{3N}\xi \exp\left\{\frac{i}{\hbar}\langle p|\xi\rangle\right\}\sum_P(-1)^P \exp\left\{-\frac{\pi}{\lambda^2}\left|Pq-q\right|^2\right\}$$

$$\times\int\limits_{q=q(0)}^{Pq(\beta)} D^{3N}q(\tau)\exp\left(-\int_0^1 d\tau\left[\frac{\pi}{\lambda^2}\sum_{a=1}^{N}\dot{q}_a^{\,2}(\tau)+\beta U\big(q(\tau)+\xi(\tau-1/2)\big)\right]\right)$$

$$\times\exp\left\{-\frac{\pi}{2\lambda^2}\langle\xi|P+E|\xi\rangle\right\}$$



1. Antisymmetrization   2. Complex - valued integrals

1. Antisymmerization and Pauli blocking.
Pair exchange pseudopotential in the phase space.

$$U\left(q+\xi\left(\tau-1/2\right)\right)\approx U\left(q\right)+\left(\tau-1/2\right)\xi_{a,i}\cdot\frac{\partial U}{\partial q_{a,i}}+$$

$$+\frac{1}{2}\left(\tau-1/2\right)^2\xi_{a,i}\xi_{b,j}\cdot\frac{\partial^2 U}{\partial q_{a,i}\partial q_{b,j}}$$

$$W(p,q)=\exp\left(-\beta V(p,q)\right)\int_{q=q(0)}^{q(\beta)}D^{3N}q(\tau)\exp\left(-\int_0^1 d\tau\left[\frac{\pi}{\lambda^2}\sum_{a=1}^{N}\dot{q}_a{}^2(\tau)+\beta U\left(q(\tau)\right)\right]\right)$$

$$\times\left(\det\left|\chi_{ai,bj}\right|\right)^{-1/2}\exp\left(-\frac{\beta}{2}\frac{p_{ai}\chi_{ai,bj}p_{bj}}{\sqrt{m_a m_b}}+\pi J_{ai}\chi_{ai,bj}J_{bj}\right)\times\cos\left(\frac{p_{ai}\chi_{ai,bj}J_{bj}}{\hbar}\right)$$

$$J_{ai}\left[q(\tau)\right]=\frac{\lambda}{2\pi}\int_0^\beta d\tau\left(\tau-\beta/2\right)\cdot\frac{\partial U\left(q(\tau)\right)}{\partial q_{ai}}\qquad \chi_{ai,bj}\left[q(\tau)\right]=\delta_{ai,bj}+\frac{\lambda^2}{2\pi}\int_0^\beta d\tau\left(\tau-\beta/2\right)^2\cdot\frac{\partial^2 U\left(q(\tau)\right)}{\partial q_{ai}\partial q_{bj}}$$

Fermi statistics is accounted for by pair exchange pseudopotential in phase space defined **by the identical and pair permutations.**

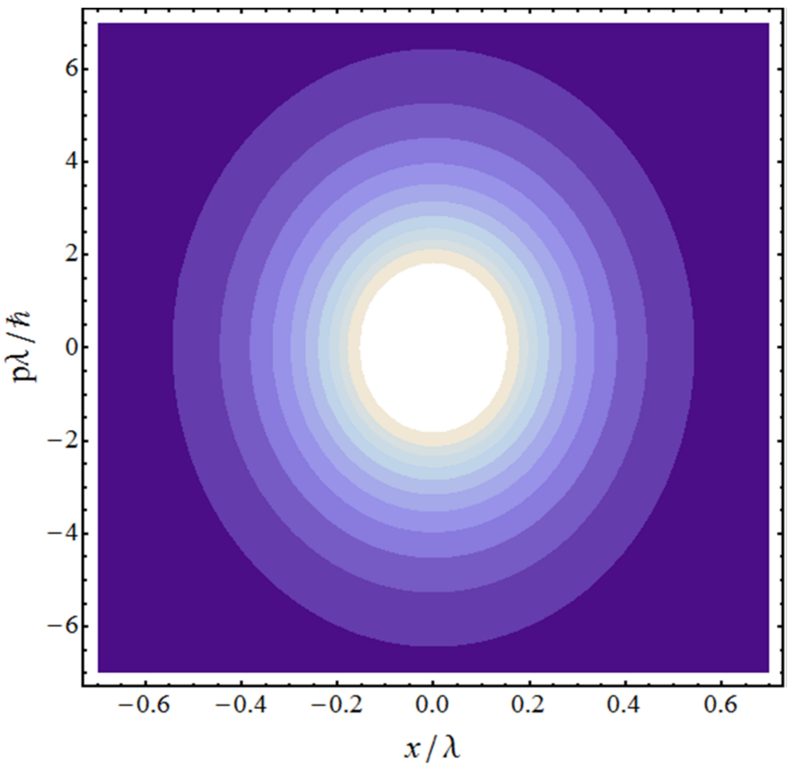
The **Pauli blocking of fermions is realized**.

$$V(p,q)=\sum_{l<t}v_{lt}\qquad v_{lt}=-kT\ln\left\{1-\exp\left(-\frac{2\pi\left|q_l-q_t\right|^2}{\lambda^2}\right)\exp\left(-\frac{\lambda^2\left|\left(p_l+J_l\right)-\left(p_t+J_t\right)\right|^2}{(2\pi h)^2\alpha(n\lambda^3)}\right)\right\}$$

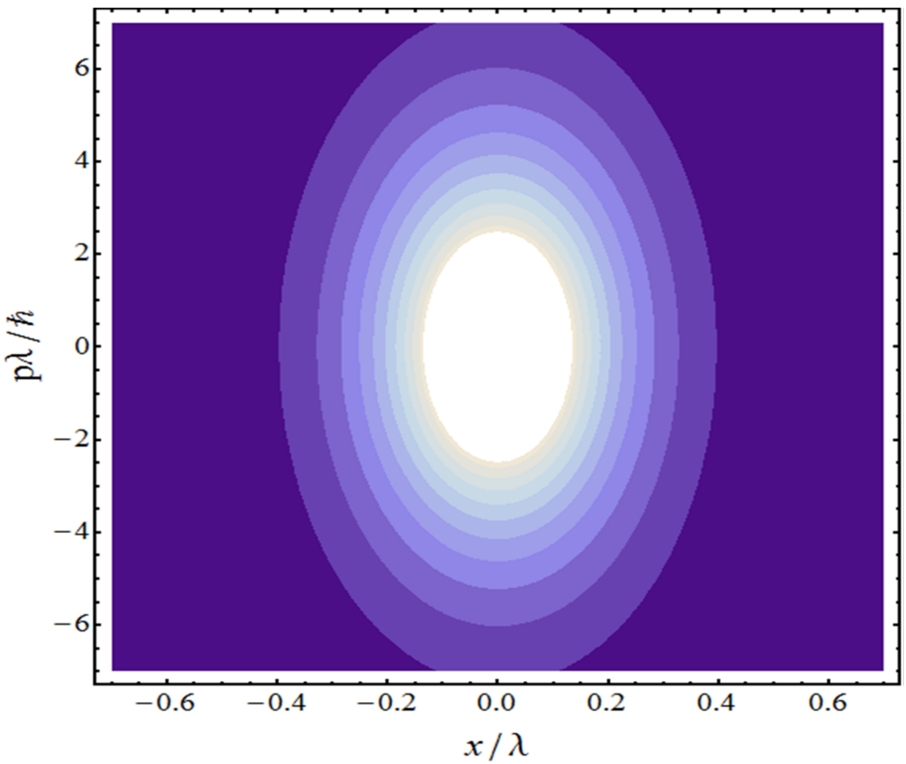
Contour plots of the repulsive effective exchange pair pseudopotentials in phase space.

In dark area pseudopotential is less than 0.1.
In white area pseudopotential is larger than 1.9.

m=1

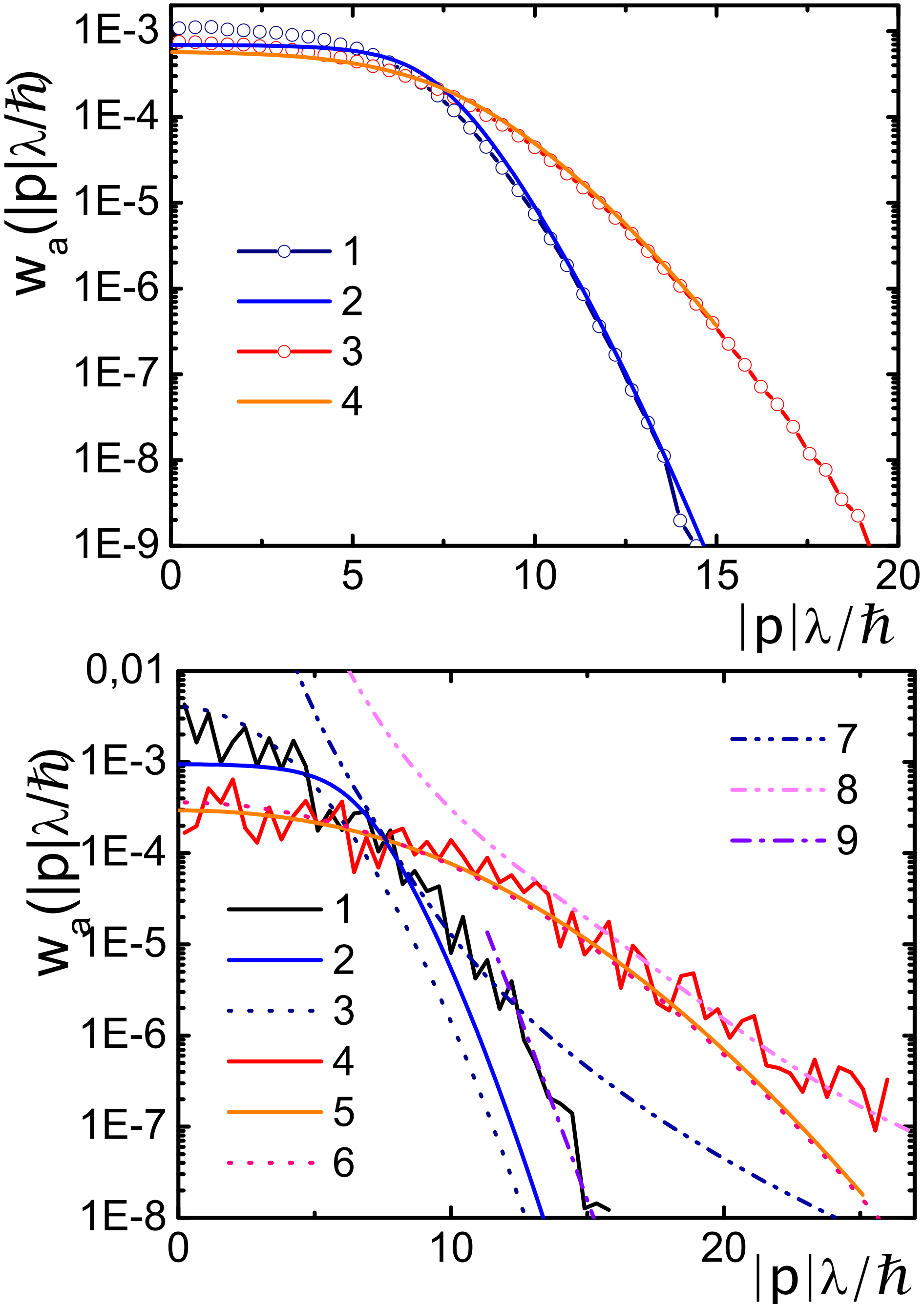


m=2



The momentum distribution functions of the ideal and strongly coupled electron-hole plasma. Holes are two times heavier than electrons. Quantum power low tails in asymptotic regions of momentum.

$$n_e \lambda^3_e \sim 5$$



2. Complex - valued path integrals and Fourier transform

$$W(p,q) = Z^{-1}\left(\frac{2\pi h\Delta\tau}{m}\right)^{-K}\int d\xi . dq_{-K} \ldots . dq_{K} \exp\left(\Phi_{2K+1}\right)$$

$$\Phi_{2K+1} = \frac{i}{h}p\xi - \frac{\Delta\tau}{h}\sum_{-K}^{K}\left[\frac{m}{2}\left(\frac{q_{k+1}-q_k}{\Delta\tau}\right)^2 + \frac{U(q_{k+1})+U(q_k)}{2}\right]$$

$$q_{-K} = q + \frac{\xi}{2}, q_K = q - \frac{\xi}{2}$$

For power dependence potential field this discrete expression consists of the following factors

$$I_k = \int_{-\infty}^{\infty} dq_k \exp\left(a_k q_k^2 + b_k q_k + c_k + d_k q_k^{\alpha}\right)$$

where integration is carried out over the real axis. The integrand is analytic, which allow us to use the Cauchy's integral theorem and deform the integration contour on the complex plane with the constant value of the integral.

Basics of the complexification on Lefschetz thimbles

Assuming that q_k takes the complex values and the action Φ is extended to a holomorphic function of q_k let us consider the set of critical points (saddle points), which satisfy condition $\partial\Phi / \partial q_k = 0$. The real Morse function in our case can be defined as $h = \Re\Phi$ and the associate gradient up/downward flows are defined by equations:

$$\frac{\partial q}{\partial l} = \pm\left(\frac{\partial \Phi}{\partial q}\right)^*$$

Intersection number n_σ of these flows $(\Pi_\sigma,.\Gamma_\sigma)$ is unity or vanishing otherwise. The Morse function h is always strictly decreasing along a downward flow. Associated with a critical point a Lefschetz thimble is defined by the union of all downward flows, which trace back to saddle point at $l \to -\infty$. Let us note that if flow equals to critical point at some l, then the flow equation implies that flow is constant for all l. So a non constant flow can only reach a critical point at $l \to -\infty$

$$I_k = \int_{-\infty}^{\infty} dq_k \exp\left(\Phi_{q(l)}\right) = \sum\nolimits_\sigma n_\sigma \exp(i\Im\Phi_{q_\sigma}) \int_{\Gamma_\sigma} Dq(l) \exp(\Re\Phi_{q(l)})$$

$$\Phi_{q(l)} = aq_k^2 + bq_k + dq_k^\alpha$$

Here n_σ is unity for intersection upflow with real axis and zero otherwise.

The Airy function

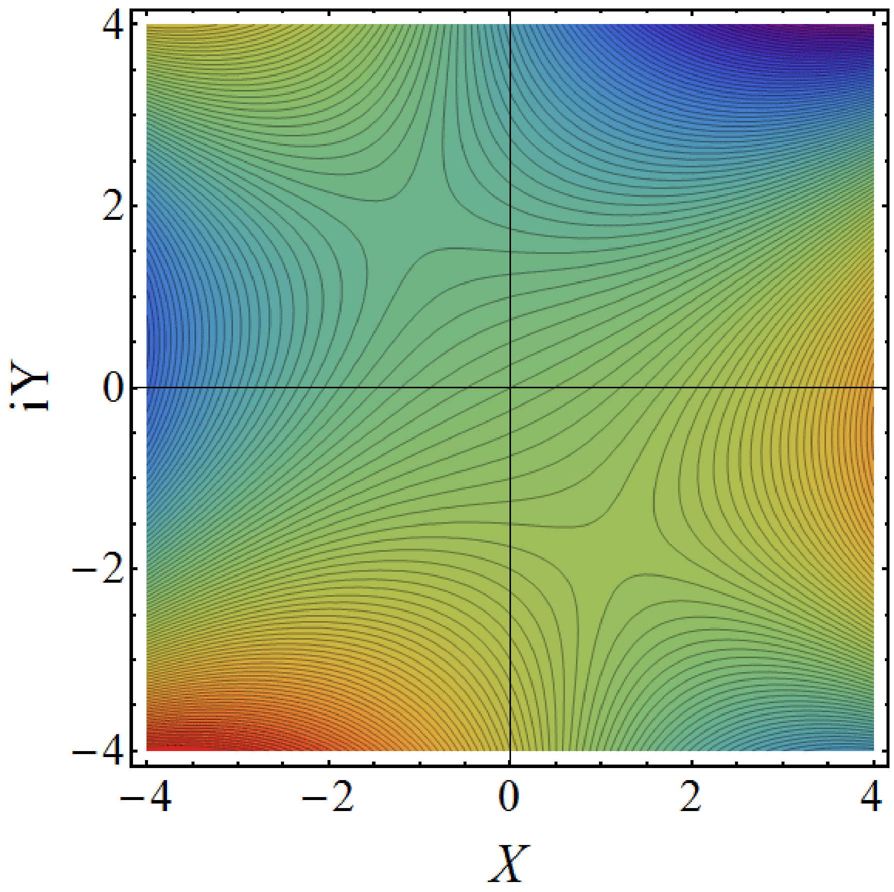
Before calculations of multidimensional integrals we have to test the algorithm proposed above by calculations of some simpler integrals with known analytical answer. It is reasonable to begin with consideration of low dimensional integrals of complex – valued strongly oscillating functions. As the first example, we consider calculation of Airy function, defined as the following integral over the real axis:

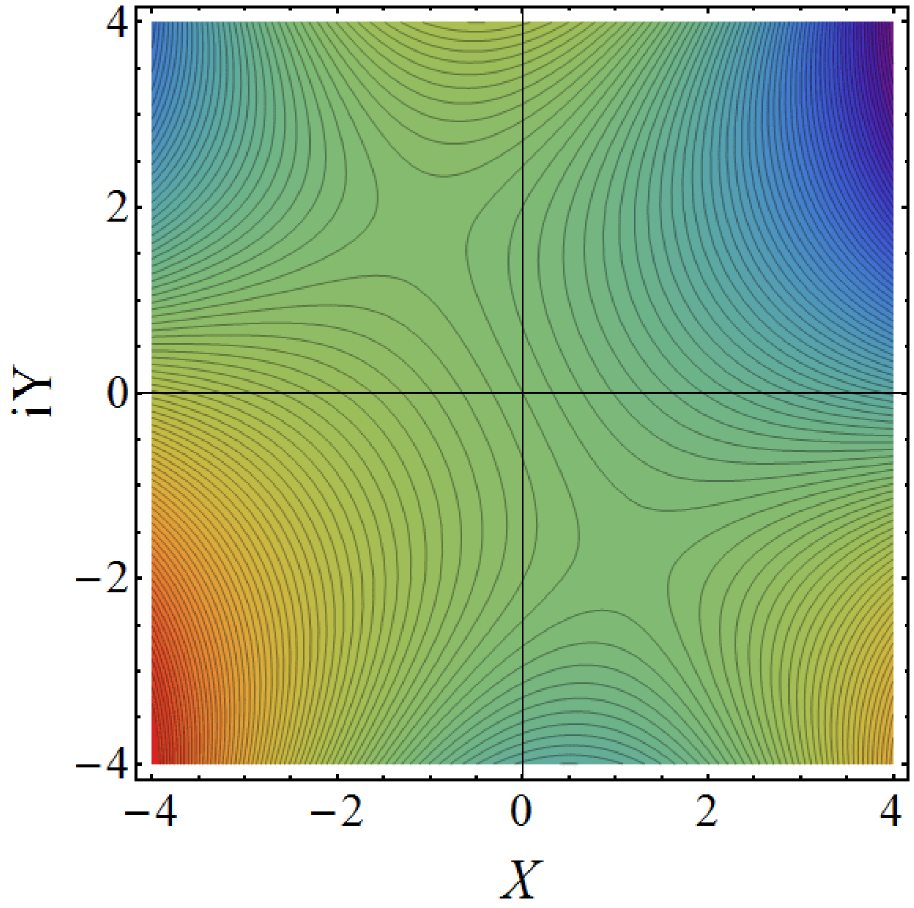
$$Ai(p) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dx \exp(i(px + x^3/3))$$

On the next slide the **critical points** are in the left upper and the right bottom quarters of the complex plane. We can deform the integration path in the complex plane of variable as long as the new path belongs to the original relative homology class, which connects regions of strongly **decaying modulus** of the integrand at infinity (blue regions).

Then the next figure shows the contour plot of the MC probability **with two red circles** at its maximum values at the critical points.

The contour plot of the imaginary part (left panel) and the real part (right panel) of the action on complex plane for p = 2 + 4i.





Metropolis – Hastings MC algorithm

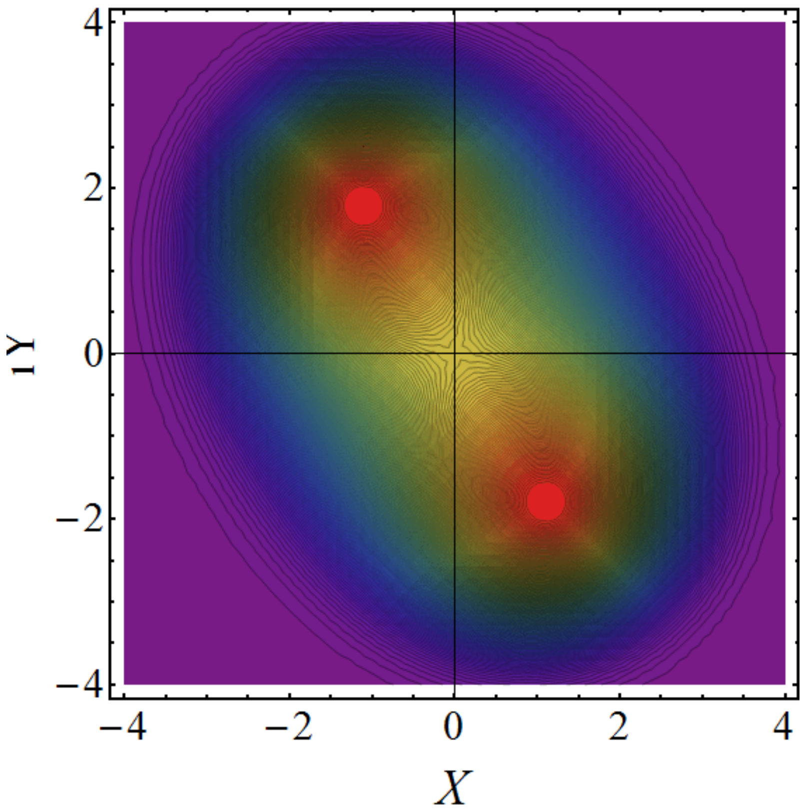
Used here MC method is based on the Metropolis – Hastings algorithm, which resides in designing a Markov process by constructing transition probabilities, such that its stationary distribution to be equal to a forgiven one. To increase efficiency of the numerical procedure we have separated the transition in two sub-steps: **the proposal and the acceptance-rejection**.

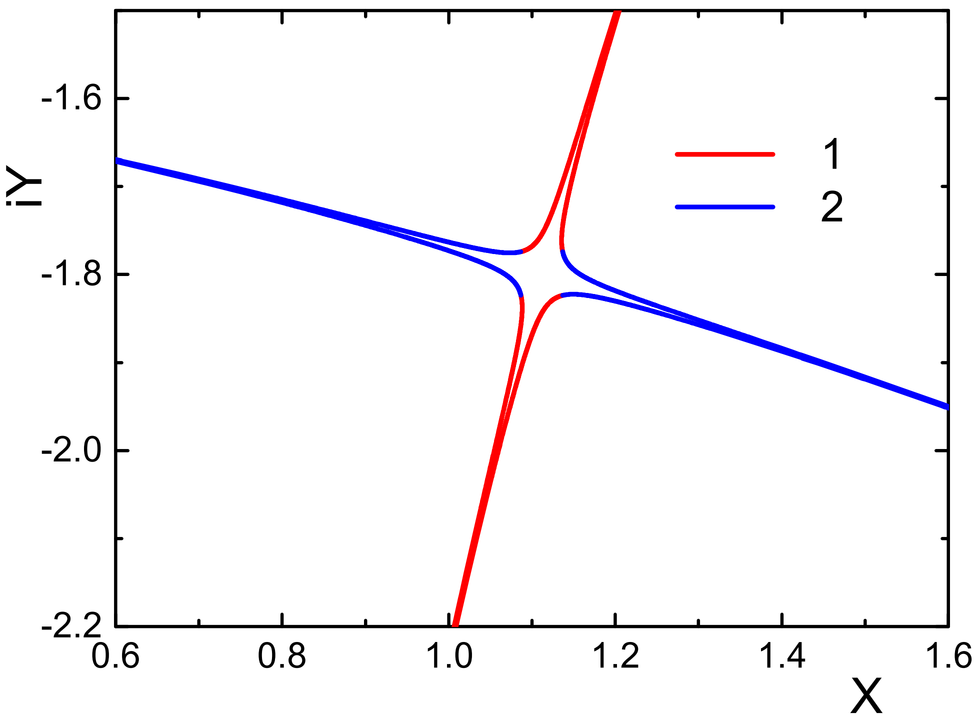
1)We are free in choosing probability proposal as it affect only the efficiency of sampling the main contribution to the integrals and does not change the final result of calculations. For optimization of the MC finding the main contribution to the integral the choice of the proposal probability may be the following $g(q \to q') = \exp(a\Re\Phi_{q'}) / \exp(a\Re\Phi_{q})$ with free appropriate fit parameter.

2)To optimize the MC search of the critical point we define the limiting probability distribution as $w(q) = \exp(-b\,|\,\partial\Phi / \partial q\,|^2)$ and the related standard Metropolis acceptance – rejection probability.

Contour plot of the probability w(q) (left panel) **and the averaged up/downward flow** (right panel).

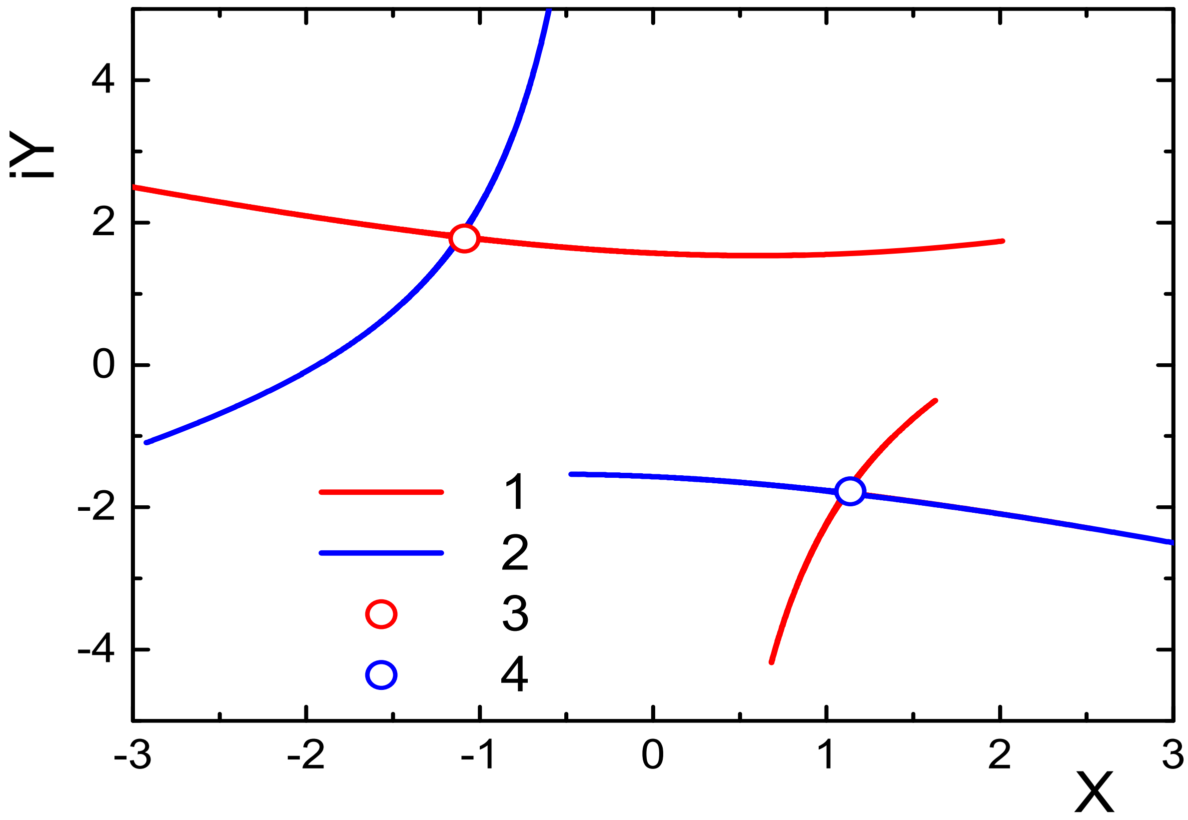
Details of initial conditions obtained by MC method in different quarters of small vicinity of the critical point





The averaged up/downward flows.

The red critical point and red associated thimbles contribute to the contour integral of the Airy function, while the blue point does not.



The MC results versus the exact Airy function

p	MC method results	Analytical Ai(p)
2+4i	0.3365 - 6.5451E-02i	0.3301 - 0.088i
0+4i	-4.8569 + 7.244i	-4.6362 + 7.4111i
4+0i	7.384E-04 + 5.65E-05i	9.515E-04 + 0i

Some discrepancies can be explained by statistical errors.

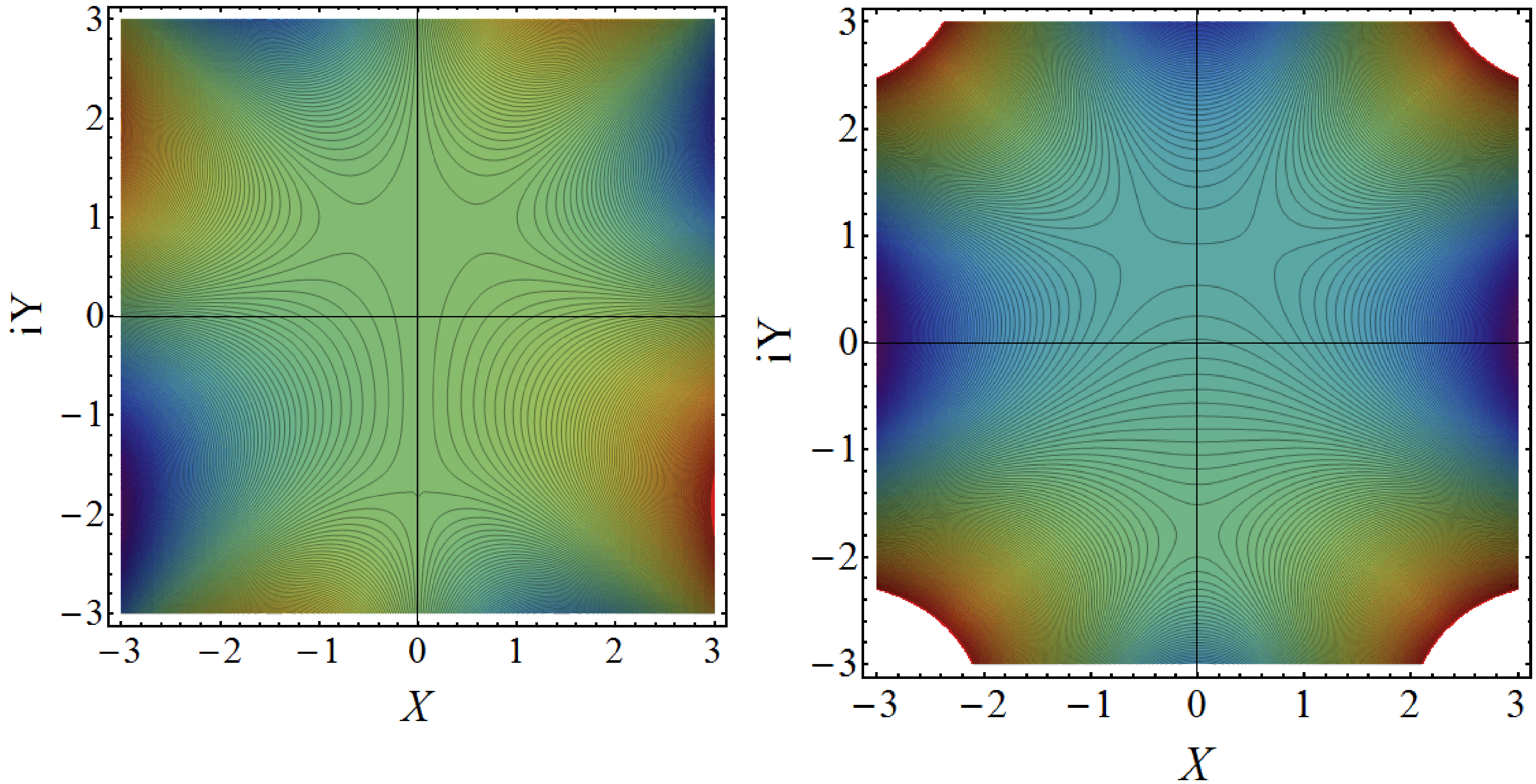
Short time path integral

Now to test the developed approach let us consider elementary factor in the finite dimensional approximation of the path integral. Factor in this approximation may be written in the form like:

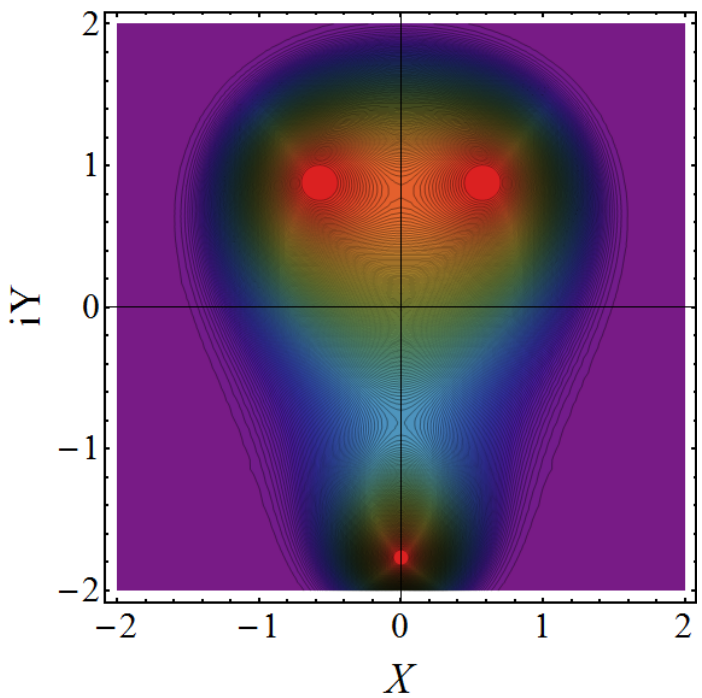
$$I_k = \int_{-\infty}^{\infty} dq_k \exp\left(i(pq + i(q - const)^2 + q^4/4)\right)$$

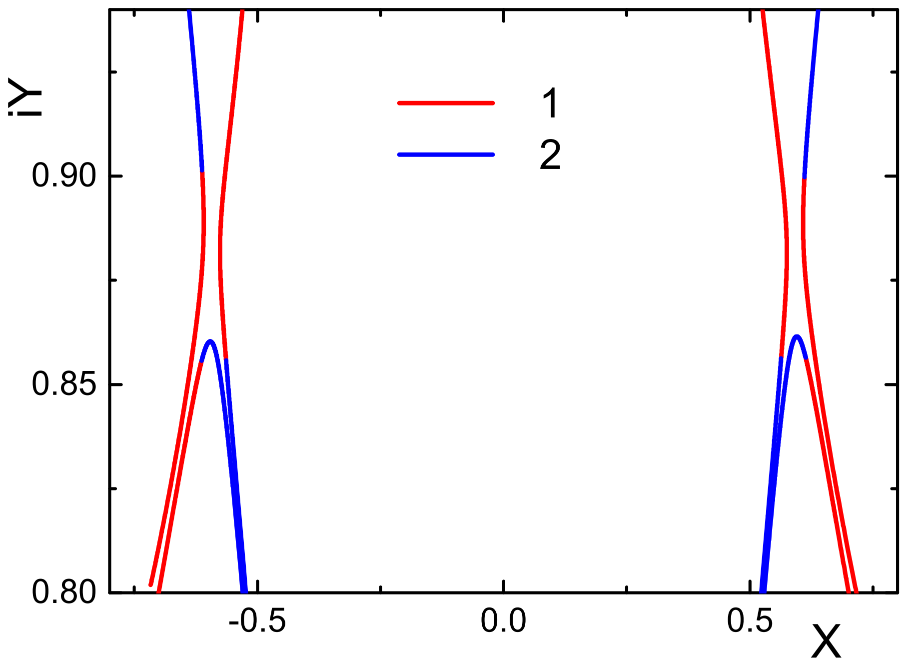
where, for example, const = 2. On the nextslides as before solution of the complex valued differential equations with MC initial conditions nearby the both upper critical points allow to obtain averaged downward (red lines) and upward (blue lines) flows. As the both blue lines for red point cross the real axis we calculate sum of the contributions to the integral along the both red Lefschetz thimbles with opposite sign due to the different thimble orientation.

The contour plot of imaginary part(left panel) and real part (right panel) of the of the power in exponent on complex plane for const = 2.



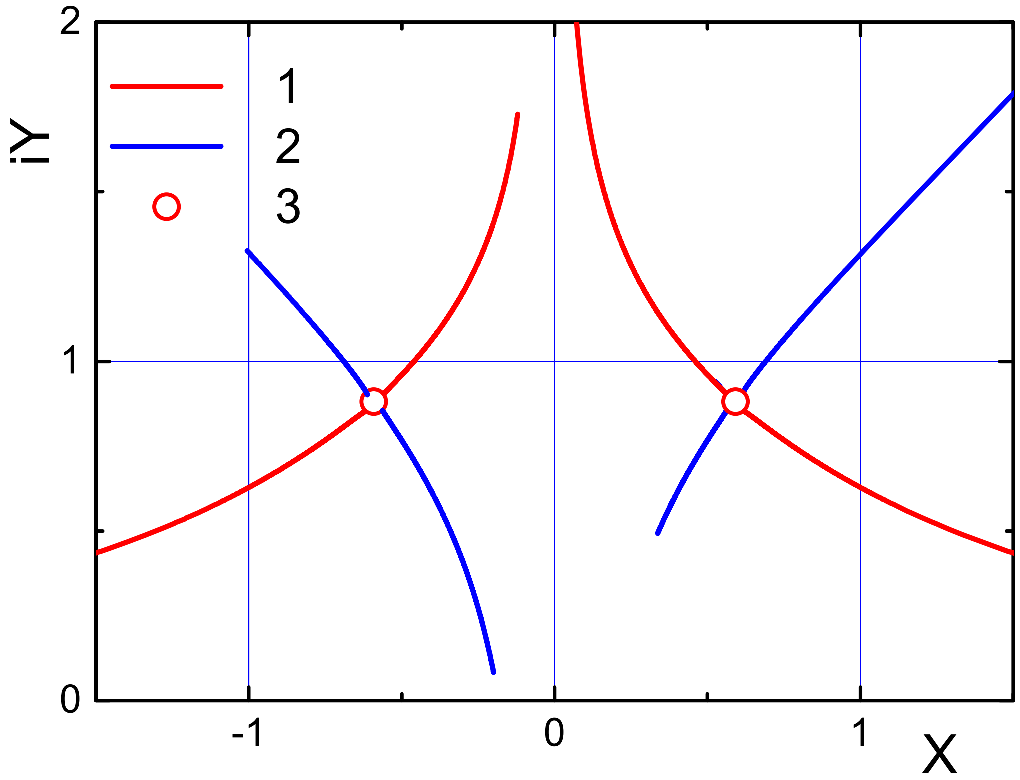
Contour plot of the probability w(q) and
details of MC initial conditions in different quarters of
small vicinity of the critical points.





The averaged downward and the upward flows .

Red critical points and the associated thimbles contribute to the contour integral
(const = 2 and p = 2+i4)



Comparison of the Monte Carlo result for Ik = 0.01306+i0.00006 with independent exact calculations Ik = 0.01402+i0 demonstrate a good enough accuracy of the developed approach.

Conclusion

Nowadays the term ’sign problem’ is used to identify two different problems.

One arises at studies of the Fermi systems by path integral approach and is caused by the requirement of **antisymmetrization** of the **real valued matrix elements** of the density matrix. To overcome this issue the new numerical version of the Wigner approach to quantum mechanics has been developed.

The ideas to overcome the ’sign problem’ of **strongly oscillating complex valued integrand** in the Feynman path integrals comes from Picard-Lefschetz theory and a complex version of Morse theory. The main idea is to select Lefschetz thimbles as the cycle approaching the saddle point at the path-integration, where the imaginary part of the complex action stays constant. and the integral can be calculated much more effectively.

Thank you for attention.

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