Kantorovich Method for Solving the Multi-dimensional Eigenvalue and Scattering Problems of Schrödinger Equation

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Abstract. A Kantorovich method for solving the multi-dimensional eigenvalue and scattering problems of Schrödinger equation is developed in the framework of a conventional finite element representation of smooth solutions over a hyperspherical coordinate space. Convergence and efficiency of the proposed schemes are demonstrated on an exactly solvable model of three identical particles on a line with pair attractive zero-range potentials below three-body threshold. It is shown that the Galerkin method has a rather low rate of convergence to exact result of the eigenvalue problem under consideration.

1 Introduction

Elaboration of stable numerical methods for the elliptic partial differential equation is one of the main problems of computational mathematics. From this point of view, the creation of numerical schemes for solving the Schrödinger equation in a multi-dimensional space is a very important task of computational physics. This is based on the fact that the numerical solution of such equation has a wide application in different quantum-mechanical problems such as the modern calculations of the weakly bound states and elastic scattering in a system of three helium atoms considered as point particles with some short range pair potentials, i.e. a trimer of helium atoms [11], and modern laser physics experiments [9]. So, the above experiments require computer modelling of dynamics of exotic few-body Coulomb systems in external laser pulse fields [7]. There are two conditions for elaborating numerical methods: to be stable and to have a high accuracy.

The main idea of this paper is to formulate Kantorovich method for solving the multi-dimensional eigenvalue and scattering problems for Schrödinger equation MSE. In this method multi-dimensional boundary problem is reduced to a system of ordinary differential equations of second order with variable coefficients on a semi-axis with the help of expansion of the solution by a set of

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orthogonal solutions of an auxiliary parametric eigenvalue problem. Then the finite-element method is applied, to construct numerical schemes for solving corresponding boundary problem for the system of ordinary differential equations with an arbitrary accuracy in the space step. Note that variable coefficients of ordinary differential equations and the corresponding solutions can have a long-range asymptotic behavior. That is why one has to be very careful in the formulation of the boundary problems under consideration. We consider as an example the known exactly solvable model of three identical particles on a line with pair attractive zero-range potentials below three-body threshold, build up adequate formulations and corresponding schemes. We verify an accuracy of these schemes in comparison with theoretical estimations, using sequences of the enclosed meshes and examine rate of convergence to exact results with respect to number of basis functions.

2 Statement of the Problem

We consider three identical particles in the local Jacobi coordinates $\{\xi,\eta\}\in R^2$ in the center-of-mass system, $\eta=2^{-1/2}(x_1-x_2)$, $\xi=6^{-1/2}(x_1+x_2-2x_3)$, where $x_i\in R^1,\ i=1,2,3$ are Cartesian coordinates of particles on a line. In polar coordinates ρ and θ, $\eta=\rho\cos\theta,\ \xi=\rho\sin\theta,\ -\pi<\theta\le\pi$, the Schrödinger equation for a partial wave function $\Psi(\rho,\theta)$ has the form:

$$\left[-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+h_\rho\right]\Psi(\rho,\theta)=\frac{2m}{\hbar^2}E\Psi(\rho,\theta). \tag{1}$$

Here E is the relative energy in the center-of-mass, $m=(m_1m_2+m_1m_3+m_2m_3)/(m_1+m_2+m_3)$ is the effective mass. We choose pair potentials $V_i(\sqrt{2}\eta)=g\delta(|\eta|)/\sqrt{2},\quad i=1,2,3$ as delta-functions of a finite strength $g=c\bar\kappa\sqrt{2}(\hbar^2/m)$, and consider an attractive case $c=-1$ and $\bar\kappa=\pi/6$, supports bound state $\phi_0(\eta)=\sqrt{\bar\kappa}\exp(-\bar\kappa|\eta|)$ with double energy $\epsilon_0^{(0)}=-\bar\kappa^2$, so that $2E=q^2+\epsilon_0^{(0)}$ in units $\hbar=m=1$, where q is a relative momentum of the pair [4]. The parametric Hamiltonian h_ρ at each fixed value $\rho\in R_+^1$ has the form (in a.e. $\hbar=\ m=1$)

$$h_\rho=-\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}+\frac{2c\bar\kappa}{\rho}\sum_{n=0}^{5}\delta(\theta-\theta_n),\ \ \theta_n=n\pi/3+\pi/6. \tag{2}$$

Using six-fold symmetric representation (2) we formulate the following boundary problem corresponding to equation (1) in the case $E<0$ [6]

$$-\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial\theta^2}\right]\Psi(\rho,\theta)=2E\Psi(\rho,\theta), \tag{3}$$

with boundary conditions by the angle variable $\theta_n\le\theta<\theta_{n+1}$

$$\begin{aligned}&\frac{1}{\rho}\frac{\partial\Psi(\rho,\theta_i)}{\partial\theta}=(-1)^{i-n}c\bar\kappa\Psi(\rho,\theta_i),\quad i=n,n+1,\quad n=0,1,...5,\\&\Psi(\rho,\theta_{n+1}-0)=\Psi(\rho,\theta_{n+1}+0),\end{aligned} \tag{4}$$

and asymptotic conditions by radial variable

$$\begin{array}{l} \lim\limits_{\rho\to 0} \rho \frac{\partial \Psi(\rho,\theta)}{\partial \rho} = 0, \\ \Psi(\rho,\theta)|_{\rho\to\infty} \to \chi_0^{as}(\rho) B_0^{as}(\rho,\theta) + F(k,\theta)\sqrt{\frac{\pi}{2k\rho}} e^{-k\rho}, k = \sqrt{-2E}. \end{array} \tag{5}$$

For a scattering problem in the open channel $E(q) > \epsilon_0^{(0)}$, i.e. for $0 < q < \bar{\kappa}$

$$\chi_0^{as}(\rho) \approx \sin(q\rho + \delta)/\sqrt{q\rho}, \tag{6}$$

where $\delta = \delta(q)$ is unknown phase shift, and for bound states ($E(q) \leq \epsilon_0^{(0)}$)

$$\chi_0^{as}(\rho) \approx e^{-\bar{q}\rho}/\sqrt{\rho}, \tag{7}$$

where $\varepsilon = \bar{q}^2 = -q^2 \geq 0$ is unknown binding energy of the three body system.

3 The Kantorovich Method

Consider a formal expansion of the solution of Eqs. (1)-(2) using the infinite set of one-dimensional basis functions $B_j(\rho;\theta) \in W_2^1(-\pi,\pi)$, $j = 0, 1, 2, \ldots$:

$$\Psi(\rho,\theta) = \sum_{j=0}^{\infty} \chi_j(\rho) B_j(\rho;\theta). \tag{8}$$

In Eq. (8), functions $\chi(\rho)^T = (\chi_0(\rho,), \chi_1(\rho), \ldots,)$ are unknown, and surface functions $B(\rho;\theta)^T = (B_0(\rho;\theta), B_1(\rho;\theta), \ldots,)$ form an orthonormal basis for each value of ρ which is treated here as a given parameter. In the Kantorovich approach [10], functions $B_j(\rho;\theta)$ are determined as solutions of the following one-dimensional parametric eigenvalue problem $\theta_n \leq \theta < \theta_{n+1}$:

$$\begin{cases} \dfrac{1}{\rho^2}\dfrac{\partial^2 B_j(\rho;\theta)}{\partial\theta^2} = -\epsilon_j(\rho) B_j(\rho;\theta), \\ \dfrac{1}{\rho}\dfrac{\partial B_j(\rho;\theta_i)}{\partial\theta} = (-1)^{n-i} c\bar{\kappa} B_j(\rho;\theta_i), \quad i = n, n+1, \quad n = 0, 1, ...5, \\ B_j(\rho;\theta_{n+1} - 0) = B_j(\rho;\theta_{n+1} + 0). \end{cases} \tag{9}$$

The eigenfunctions of this problem are normalized as follows

$$< B_i(\rho;\theta) | B_j(\rho;\theta) >= \int_{-\pi}^{\pi} B_i(\rho;\theta) B_j(\rho;\theta) d\theta = \delta_{ij}. \tag{10}$$

After substitution of expansion (8) into the Rayleigh-Ritz variational functional (see [3]) and subsequent minimization of the functional, the solution of Eqs. (1)-(2) is reduced to a solution of an eigenvalue problem for the finite set of n_{max} ordinary second-order differential equations for determining energy E and coefficients (radial wave functions) $\chi(\rho)$ of expansion (8)

$$-\mathbf{I}\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d\chi}{d\rho} + \mathbf{V}\chi - \mathbf{A}\frac{d\chi}{d\rho} - \frac{1}{\rho}\frac{d\rho\mathbf{A}\chi}{d\rho} = 2E\mathbf{I}\chi, \quad \lim_{\rho\to 0}\rho\frac{d\chi(\rho)}{d\rho} = 0. \tag{11}$$

The boundary conditions on $\rho \to \infty$ are (6) or (7) corresponding to the problem. In these expressions matrix $\mathbf{V}$ is symmetric one and $\mathbf{A}$ is anti-symmetric. They are given by the formulas

$$V_{ij} = H_{ij} + 0.5(\epsilon_i + \epsilon_j)\delta_{ij}, \quad H_{ij}(\rho) = \left\langle \frac{\partial}{\partial\rho} B_i(\rho;\theta) \left| \frac{\partial}{\partial\rho} B_j(\rho,\theta) \right.\right\rangle, \qquad A_{ij}(\rho) = \left\langle B_i(\rho;\theta) \left| \frac{\partial}{\partial\rho} B_j(\rho;\theta) \right.\right\rangle. \tag{12}$$

As is shown in paper [8] the problem (9) - (10) has analytical solutions

$$\begin{aligned} B_0(\rho;\theta) &= \sqrt{\frac{y_0^2 - x^2}{\pi(y_0^2 - x^2) + |x|}} \cosh\left[6y_0(\theta - n\pi/3)\right], \\ B_j(\rho;\theta) &= \sqrt{\frac{y_j^2 + x^2}{\pi(y_j^2 + x^2) - |x|}} \cos\left[6y_j(\theta - n\pi/3)\right], \\ \epsilon_0(\rho) &= -\left(\frac{6y_0(\rho)}{\rho}\right)^2, \quad \epsilon_j(\rho) = \left(\frac{6y_j(\rho)}{\rho}\right)^2. \end{aligned} \tag{13}$$

The functions $\epsilon_0(\rho), \epsilon_j(\rho), j = 1, 2, \ldots$ can be calculated as the roots of transcendental equations, which follow from the boundary problems (9)-(10) at c=-1,

$$\begin{aligned} y_0(\rho)\tanh(\pi y_0(\rho)) = -x,\ 0 \le y_0(\rho) < \infty,\quad x = c\tfrac{\pi}{36}\rho, \\ y_j(\rho)\tan(\pi y_j(\rho)) = x,\ j - \tfrac{1}{2} < y_j(\rho) < j,\ j = 1, 2, 3, ... \end{aligned} \tag{14}$$

So using analytical expressions for functions $B_0, \epsilon_0,\ \ B_j, \epsilon_j$ we have a possibility to calculate the matrix elements $V_{ij},\ \ A_{ij}$ analytically.

4 The Galerkin Method

Let us consider the following expansion for the wave function $\Psi(\rho, \theta)$

$$\Psi(\rho, \theta) = \frac{1}{\sqrt{2\pi}}\bar{\chi}_0(\rho) + \frac{1}{\sqrt{\pi}}\sum_{j=1}^{\infty}\bar{\chi}_j(\rho)\cos(6j\theta). \tag{15}$$

In this expansion the basic function $\eta_j(\theta)$ are solutions of the eigenvalue problem $-\dfrac{d^2b}{d\theta^2} = \bar{\epsilon}\rho^2 b$ with six-fold symmetry conditions and functions $\bar{\chi}_j(\rho)$ are unknown coefficients. In this case we have that $b_j(\theta) = \cos(6j\theta)$. Using these functions the corresponding matrix elements in the system of radial equations (12) have the form

$$H_{ij}(\rho) = \begin{cases} c/\rho, \text{ if } i = j = 0, \\ (-1)^j\sqrt{2}c/\rho, \text{ if } i = 0,\ j \neq 0, \\ (-1)^i\sqrt{2}c/\rho, \text{ if } i \neq 0,\ j = 0, \\ (-1)^{i+j}2c/\rho, \text{ if } i \neq 0,\ j \neq 0, \end{cases} \tag{16}$$

$$A_{ij}(\rho) = 0,\ V_{ij}(\rho) = H_{ij}(\rho) + 0.5(\bar{\epsilon}_i(\rho) + \bar{\epsilon}_j(\rho))\delta_{ij},\ \bar{\epsilon}_i(\rho) = (6i/\rho)^2. \tag{17}$$

Below we will compare the convergence of the Kantorovich method and the Galerkin method on example of a calculation for the ground state of the discrete spectrum problem under consideration.

5 Reducing the Problem to a Finite Interval

We consider a reduction the boundary problem from semi-axis to finite interval using known asymptotic behavior of variable coefficients $H_{ij}(\rho)$, $A_{ij}(\rho)$ and $\varepsilon_j(\rho)$ and solutions $\chi_j(\rho)$ at small and large values of radial variable ρ.

5.1 Discrete Spectrum Problem

In the paper [6] the following asymptotics for components $\chi_0(\rho), \chi_1(\rho), \ldots$ are hold

$$\chi_0(\rho) \approx \frac{\exp(-\bar{q}\rho)}{\sqrt{\rho}}, \quad \chi_j(\rho) \approx \sqrt{\frac{\pi}{2k\rho}} \exp(-k\rho),\ j = 1, 2, \ldots. \tag{18}$$

From these relations we can obtain the homogeneous third type boundary condition for large $\rho_m, \rho_m >> 1,\ j = 1, 2, \ldots$

$$\rho_m \frac{d\chi_0(\rho_m)}{d\rho} = -(\frac{1}{2} + \bar{q}\rho_m)\chi_0(\rho_m),\ \rho_m \frac{d\chi_j(\rho_m)}{d\rho} = -(\frac{1}{2} + k\rho_m)\chi_j(\rho_m). \tag{19}$$

Here $\bar{q}^2 = -2E - \pi^2/36 \geq 0$, where $E < 0$ is the unknown eigenvalue. So the problem has to be nonlinear. But in the considered case we can use for simplicity its known analytical value ($-2E^b_{exact} = \pi^2/9$ for a ground state, $-2E^{hb}_{exact} = \pi^2/36$ for a half-bound state) and the problem becomes a linear one.

5.2 Continuous Spectrum Problem

In this case the asymptotics of functions $\chi_j,\ j = 0, 1, \ldots$ for large ρ are

$$\begin{aligned}
\chi_0(\rho)\Big|_{\rho\to\infty} &\to J_0(q\rho) - \tan\delta' Y_0(q\rho) \\
&= \sqrt{\tfrac{2}{q\pi\rho}}\left(\sin\left(q\rho + \tfrac{\pi}{4}\right) + \tan\delta' \cos\left(q\rho + \tfrac{\pi}{4}\right)\right) + O(\rho^{-3/2}), \\
\chi_j(\rho)\Big|_{\rho\to\infty} &\to (\epsilon_0(\rho) - \epsilon_j(\rho))^{-1}\left[-A_{j0}(\rho)\frac{d}{d\rho} - \frac{1}{\rho}\frac{d}{d\rho}\rho A_{j0}(\rho) + H_{j0}(\rho)\right]\chi_0(\rho).
\end{aligned} \tag{20}$$

Now we have the following nonhomogeneous third type boundary conditions for given value of $0 < q < \bar{\kappa},\ \ 2E = q^2 - \dfrac{\pi^2}{36} < 0$

$$\rho \frac{d\chi_0(\rho)}{d\rho}\Big|_{\rho=\rho_m} = \rho\left(\frac{dJ_0(q\rho)}{d\rho} - \tan\delta' \frac{dY_0(q\rho)}{d\rho}\right)\Big|_{\rho=\rho_m}, \tag{21}$$

$$\tan(\delta') = \frac{\pi}{2}\int_0^{\rho_m} J_0(q\rho)V_0(\rho)\chi(\rho)\rho d\rho,\ \delta = \frac{\pi}{4} - \delta' + \pi. \tag{22}$$

Here $\delta = \delta(q)$ is the value of the required phase shift at a fixed value of momentum $0 < q < \pi/6$ and $J_0(\rho)$ and $Y_0(\rho)$ are the cylindrical Bessel functions of the first and second king, and

$$V_0(\rho)\chi(\rho) = \sum_{j=1}^{\infty}\left(-A_{0j}(\rho)\frac{d}{d\rho} - \frac{1}{\rho}\frac{d}{d\rho}\rho A_{0j}(\rho) + H_{0j}(\rho)\right)\chi_j(\rho) + \left(V_{00}(\rho) + \frac{\pi^2}{36}\right)\chi_0(\rho). \tag{23}$$

For high accuracy calculation of $\tan(\delta')$ we take into account asymptotic correction terms in an exact definition of the phase shift

$$\tan(\delta') = \frac{\pi}{2}\int_0^{\rho_m} J_0(q\rho)V_0(\rho)\chi(\rho)\rho d\rho + v^{as} - \tan(\delta')u^{as}. \tag{24}$$

As a result we have the following formula

$$\tan(\delta') = \left(\frac{\pi}{2}\int_0^{\rho_m} J_0(q\rho)V_0(\rho)\chi(\rho)\rho d\rho + v^{as}\right)/(1+u^{as}), \tag{25}$$

where the asymptotic correction terms are of the form

$$\begin{aligned} v^{as} &= \tfrac{\pi}{2}\textstyle\int_{\rho_m}^{\infty} J_0(q\rho)\left(V_{00}(\rho) + \tfrac{\pi^2}{36}\right)J_0(q\rho)\rho d\rho \sim O\left(\tfrac{1}{\rho_m}\right), \\ u^{as} &= \tfrac{\pi}{2}\textstyle\int_{\rho_m}^{\infty} J_0(q\rho)\left(V_{00}(\rho) + \tfrac{\pi^2}{36}\right)Y_0(q\rho)\rho d\rho \sim O\left(\tfrac{1}{\rho_m^2}\right). \end{aligned} \tag{26}$$

Here the exact value of the phase shift δ for each $q \in (0, \pi/6)$ equals

$$\delta_{exact} = \frac{3\pi}{2} - \arctan\frac{8\sqrt{3}q\pi}{\pi^2 - 36q^2}. \tag{27}$$

6 Numerical Method

For numerical solution of one-dimensional eigenvalue problems and boundary value problem (11) subject to the corresponding boundary conditions (6) and (7), the high-order approximations of the finite element method [12,5] elaborated in our previous papers [3,1,2] have been used. One-dimensional finite elements of order $p = 1, 2, \ldots, 10$ have been implemented. Using the standard finite element procedures [5], these problems are approximated by the generalized algebraic eigenvalue problem

$$\mathbf{K}\mathbf{F}^h = E^h\mathbf{M}\mathbf{F}^h. \tag{28}$$

and the system of linear algebraic equations

$$\hat{\mathbf{K}}\mathbf{u}^h = \mathbf{U}. \tag{29}$$

Here $\mathbf{K}$ and $\mathbf{M}$ are the standard stiffness and mass matrices, corresponding to discrete spectrum problem, matrix $\hat{\mathbf{K}}$ and right-hand side vector $\mathbf{U}$ correspond to continuous spectrum problem, E^h and $\mathbf{F}^h$ are the numerical approximation of the corresponding eigenvalue problem and $\mathbf{u}^h$ is the finite element approximation of the continuous wave function on the finite-element grid.

7 Numerical Results

Here we study the convergence rate of the Kantorovich and Galerkin methods (KM and GM) in depending on a number of equations of system (11). The problem under consideration is a good test for numerical methods because it has analytical solutions of discrete and continuous spectrum. First we consider the eigenvalue problem with $\rho_m = 50$. We use the 1000 finite elements of forth order. The finite element grid consists 4001 nodes. We consider the calculations with double and quadruple precision for the KM and double precision of the GM. In Table 1 the differences $\Delta E = -2E^h + 2E^{exact}$ for each case are shown. One can see that if we use the quadruple precision the KM monotonically converges to the exact values while for double precision calculations it holds true only till 35 equations. Note that for the solution of algebraic eigenvalue problem we apply the Subspace iteration method. The main step there is to find the solutions of system of linear algebraic equations with matrix K using the Cholesky decomposition. For $N = 50$ this system consists of 200050 equations. It can be solved stable only if we use the quadruple precision. The last column shows that there is a rather low rate of convergence for the GM, because it is compatible with boundary conditions only in vicinity of small values ρ. So, the GM it can not apply in the scattering problem. For scattering problem we calculate phase shift δ^h at $q\rho_m = 300$ and use 1500 finite elements of forth order. The finite element grid consists 6001 nodes. In Table 2 differences $\Delta\delta = \delta^{exact} - \delta^h$ are shown. One can see that the KM converges monotonically to the exact values δ^{exact} with a rate of order 1/N.

Table 1. The convergence of the Kantorovich method (KM) for the differences $\Delta E = -2E^h + 2E^{exact}$ of energy value of the ground state versus the number of equations. First column shows the number of equations N, second and fourth ones display the accuracy of calculations for quadruple and double precision. Sixth column shows a rather low rate of convergence of the Galerkin method (GM). Thirds, fifth and seventh columns shows correspondingly CPU times for calculations on PC III-750MHz

N	ΔE_{KM}^{quad}	CPU^{quad}	ΔE_{KM}^{double}	CPU^{double}	ΔE_{GM}^{double}	CPU^{double}
1	1.801(-04)	0.225	1.801(-04)	0.023	9.662(-2)	0.020
2	2.762(-06)	1.169	2.762(-06)	0.082	4.116(-2)	0.046
3	2.697(-07)	2.791	2.697(-07)	0.183	2.573(-2)	0.083
4	5.413(-08)	5.142	5.413(-08)	0.325	1.866(-2)	0.154
5	1.594(-08)	8.414	1.594(-08)	0.515	1.462(-2)	0.220
6	5.949(-09)	11.978	5.950(-09)	0.770	1.201(-2)	0.336
10	3.967(-10)	33.765	3.979(-10)	2.194	7.010(-3)	0.880
20	1.099(-11)	137.805	1.245(-11)	8.273	3.431(-3)	3.448
30	1.390(-12)	303.616	3.276(-12)	18.222	2.271(-3)	8.096
35	6.357(-13)	430.993	3.194(-12)	24.608	1.943(-3)	11.556
40	3.232(-13)	571.624	3.361(-12)	31.970	1.697(-3)	15.457
50	1.046(-13)	916.614	4.427(-12)	52.430	1.355(-3)	26.433

Table 2. The differences $\Delta\delta = \delta^{exact} - \delta^{h}$ of exact and numerical results (with the double precision) of phase shift versus the number of equations N and momentum q.

N	q					
	0.002	0.100	0.200	0.300	0.400	0.500
1	6.180(-1)	2.972(-2)	3.946(-2)	3.311(-2)	6.857(-2)	8.513(-2)
2	2.991(-2)	5.716(-3)	1.038(-2)	1.548(-2)	2.064(-2)	2.583(-2)
3	5.279(-3)	3.011(-3)	5.920(-3)	8.869(-3)	1.182(-2)	1.478(-2)
4	1.706(-3)	2.074(-3)	4.128(-3)	6.188(-3)	8.250(-3)	1.031(-2)
5	7.554(-4)	1.587(-3)	3.165(-3)	4.746(-3)	6.329(-3)	7.914(-3)
6	4.034(-4)	1.285(-3)	2.566(-3)	3.848(-3)	5.131(-3)	6.417(-3)
10	8.353(-5)	7.303(-4)	1.459(-3)	2.188(-3)	2.918(-3)	3.662(-3)
16	2.567(-5)	4.435(-4)	8.863(-4)	1.329(-3)	1.774(-3)	2.273(-3)
20	1.627(-5)	3.518(-4)	7.031(-4)	1.054(-3)	1.410(-3)	1.858(-3)

8 Conclusions

The stably numerical schemes for solving MSE with high accuracy with respect to variables ρ are developed. New results are obtained for the long-range potential MSE by using PC without essential computer resources (see Table 1). It is shown that the obtained numerical results strongly correspond to the theoretical ones. This paper opens the way to apply elaborated methods for solving the MSE for the system of second-order ordinary differential equations and realizing the Kantorovich method for multi-dimensional problems [3].

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