Finite-difference splitting scheme for three-dimensional Schrödinger equation, describing tunneling from anharmonic atomic traps

I.S. Ishmukhamedov[a,b], V.S. Melezhik[a,c]

[a] *Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, Russia*
[b] *Al-Farabi Kazakh National University, Almaty, Kazakhstan*
[c] *Dubna State University, Dubna, Russia*

Overview

Why is it interesting?

- Tunneling occurs in nuclear physics (e.g. α-decay). In the scanning microscopy the tunneling of electrons is used for imaging of materials.

- Tunneling in atomic (optical) traps: a tunneling rate (experimentally measurable parameter) gives an information about effective interaction between atoms and a population of quantum states.

- 1) S.E. Gharashi and D. Blume, (2015) *Tunneling dynamics of two interacting one-dimensional particles*, Physical Review A 92, 033629 ;
2) M. Rontani, (2013) *Pair tunneling of two atoms out of a trap*, Physical Review A 88, 043633 ;

  3) S. Hunn, K. Zimmermann, M. Hiller, and A. Buchleitner, (2013) *Tunneling decay of two interacting bosons in an asymmetric double-well potential: A spectral approach*, Phys. Rev. A 87, 043626

Operator Splitting Method for the 2D Schrödinger equation

$$i\frac{\partial\psi(x_1,x_2,t)}{\partial t} = H\psi(x_1,x_2,t). \tag{1}$$

$$\psi(x_1,x_2,t+\Delta t) = e^{-i\Delta t H}\psi(x_1,x_2,t). \tag{2}$$

$$H = H_1(x_1) + H_2(x_2) + V_{\rm int}(x_1 - x_2), \tag{3}$$

$$H_j(x_j) = -\frac{1}{2}\frac{\partial^2}{\partial x_j^2} + V^{(\rm sw)}(x_j) \tag{4}$$

$$\boxed{e^{-i\Delta t H} = e^{-i\frac{\Delta t}{2}V_{\rm int}(x_1-x_2)}e^{-i\Delta t H_1(x_1)}e^{-i\Delta t H_2(x_2)}e^{-i\frac{\Delta t}{2}V_{\rm int}(x_1-x_2)} + \mathcal{O}(\Delta t^3)} \tag{5}$$

$$\psi(x,t+\Delta t) = e^{-iH_j\Delta t}\psi(x,t) \approx \left(1+\frac{1}{2}iH_j\Delta t\right)^{-1}\left(1-\frac{1}{2}iH_j\Delta t\right)\psi(x,t) \tag{6}$$

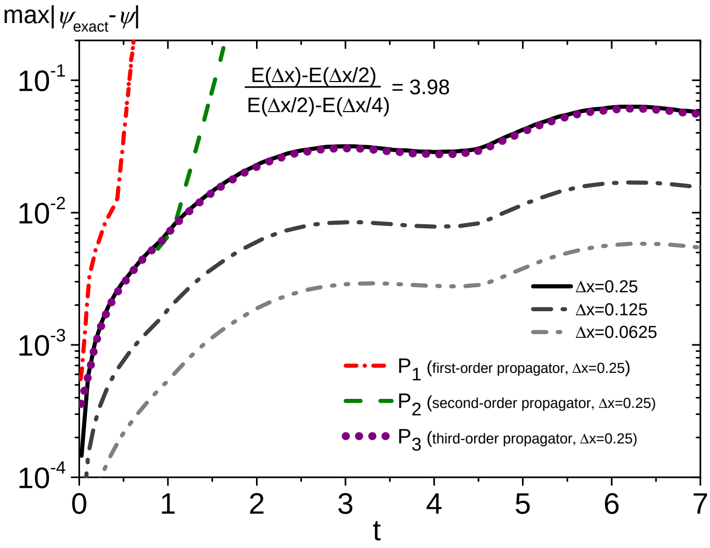
1D Schrödinger equation

$$i\frac{\partial\psi(x,t)}{\partial t} = H\psi(x,t). \tag{7}$$

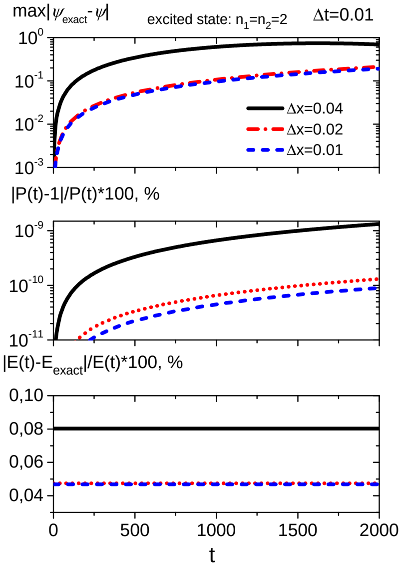
$$\psi(x,t+\Delta t) = e^{-iH\Delta t}\psi(x,t) \approx \left(1+\frac{1}{2}iH\Delta t\right)^{-1}\left(1-\frac{1}{2}iH\Delta t\right)\psi(x,t) \tag{8}$$

1D Harmonic Oscillator: comparison with a direct method

I. Gonoskov and M. Marklund, *Single-step propagators for calculation of time evolution in quantum systems with arbitrary interactions*, Comp. Phys. Comm. **202**, 211-215, (2016)



2D Harmonic Oscillator: comparison with the exact solution



$$P(t) = \int\int dx_1 dx_2 |\psi(x_1, x_2, t)|^2$$

$$E(t) = \langle \psi(x_1, x_2, t) \frac{\partial \psi(x_1,x_2,t)}{\partial t} \rangle$$

2D Harmonic Oscillator: confirmation of the theoretical estimate

Δx	Energy level, E	Ratio$= \frac{E(\Delta x)-E(\Delta x/2)}{E(\Delta x/2)-E(\Delta x/4)}$
0,2	4,997627402004	62,01651426
0,1	4,997656385391	63,49719011
0,05	4,997656852741	64,14630068
0,025	4,997656860101	
0,0125	4,997656860216	

Δt	Energy level, E	Ratio$= \frac{E(\Delta t)-E(\Delta t/2)}{E(\Delta t/2)-E(\Delta t/4)}$
0,08	4,852465011	3,938312842
0,04	4,96265524	3,984426277
0,02	4,990634284	3,996096962
0,01	4,997656385	3,999023639
0,005	4,999413625	
0,0025	4,999853043	

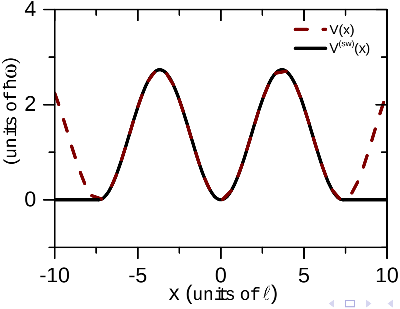
Tunneling of two interacting bosonic atoms

[Energy in $\hbar\omega$ units, length in $\ell = \sqrt{\frac{\hbar}{m\omega}}$ units. $m_1 = m_2 = m$.]

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + V^{(\mathrm{sw})}(x_1) + V^{(\mathrm{sw})}(x_2) + V_{\mathrm{int}}(x_1 - x_2) \tag{9}$$

where $V^{(\mathrm{sw})}(x_j)$ - is a potential describing the interaction of the atoms with the trap:

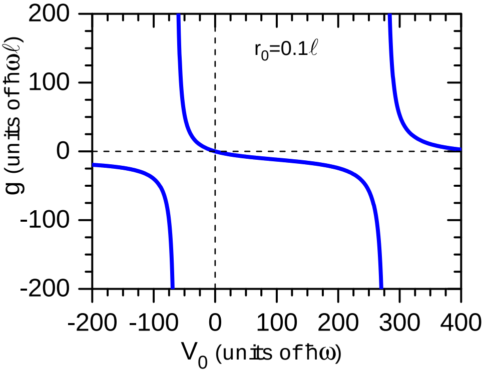
$$V^{(\mathrm{sw})}(x_j) = \begin{cases} V(x_j) = -\frac{\hbar\omega}{12\alpha}\sin^2\left(\sqrt{-6\alpha}\frac{x_j}{\ell}\right), & |x_j| \leq \frac{\pi\ell}{\sqrt{-6\alpha}} \\ 0, & |x_j| > \frac{\pi\ell}{\sqrt{-6\alpha}} \end{cases}$$
$$j = 1, 2 \tag{10}$$



Free-space scattering. Separation of the center-of-mass and relative motions

$$\left[-\frac{d^2}{dx^2} - V_0 \exp\left\{-\frac{x^2}{2r_0^2}\right\}\right]\psi_{\rm rel}(x) = k^2\psi_{\rm rel}(x), \qquad x = x_1 - x_2, \tag{11}$$

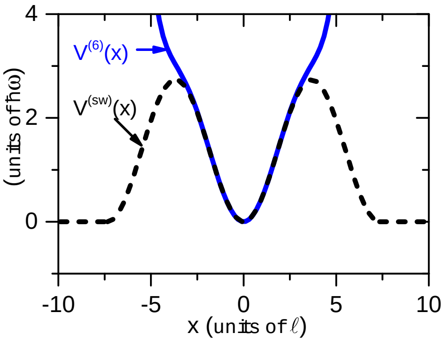
$$\psi_{\rm rel}(x) \xrightarrow[x\to\pm\infty]{} \cos(k|x| + \delta(k)) \qquad a = \lim_{k\to 0} \frac{\cot(\delta(k))}{k}, \qquad g = -\frac{2}{a}$$



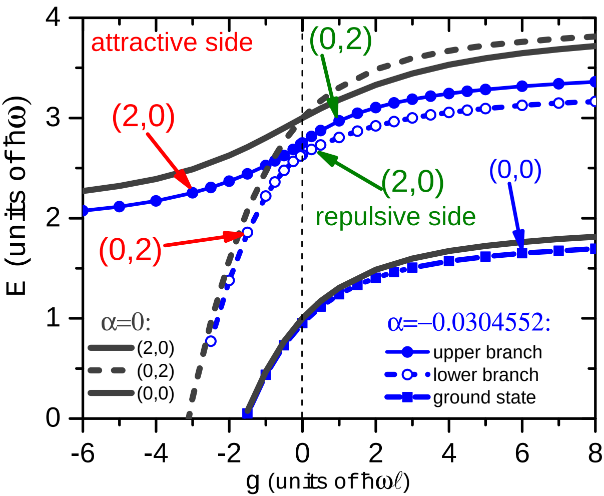
Preparation of an initial state

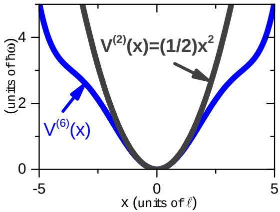
$$H = -\frac{1}{2}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + V^{(6)}(x_1) + V^{(6)}(x_2) + V_{\rm int}(x_1 - x_2) \tag{12}$$

$$V^{(6)}(x) = \frac{1}{2}x^2 + \alpha x^4 + \frac{4\alpha^2 x^6}{5} - \text{"closed" trapping potential} \tag{13}$$



Energy spectrum





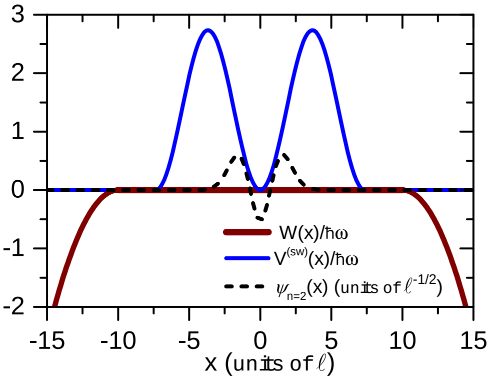
Complex Absorbing Potential (CAP)

$$H \Rightarrow H + iW(x_1) + iW(x_2), \qquad (14)$$

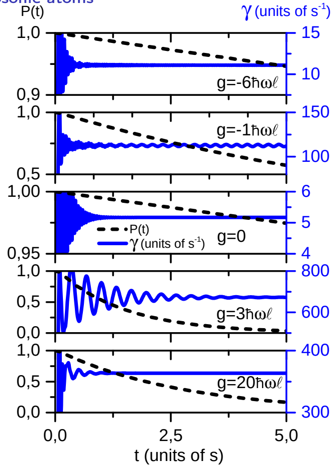
where

$$W(x_j) = w_c(|x_j| - x_c)^2\theta(|x_j| - x_c) \qquad (15)$$

where $\theta(x)$ - is the Heaviside step function.



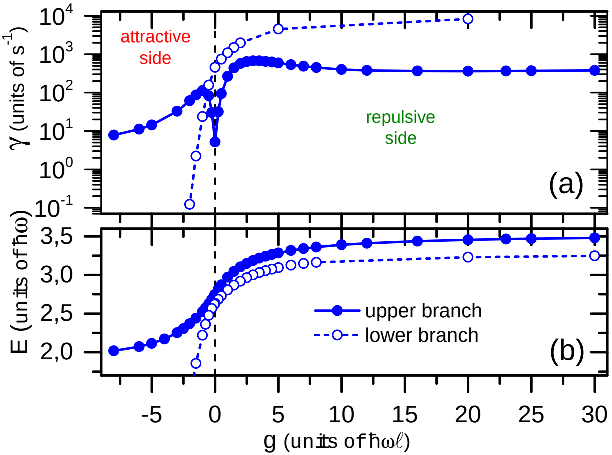
Tunneling rates



survival probability $$P(t) = \int_{-x_{\mathbf{max}}}^{x_{\mathbf{max}}} \int_{-x_{\mathbf{max}}}^{x_{\mathbf{max}}} dx_1 dx_2 |\psi(x_1, x_2, t)|^2 \sim \exp\{-\gamma t\} \qquad (16)$$

tunneling rate $$\gamma = -\frac{1}{P(t)} \frac{dP(t)}{dt}, \qquad (17)$$

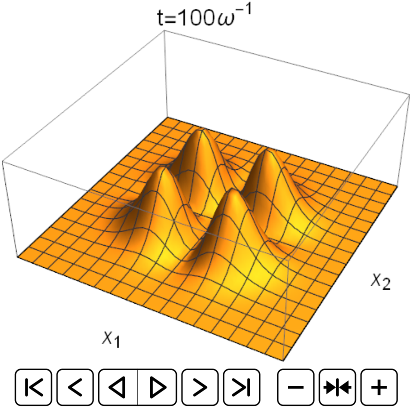
Tunneling rates



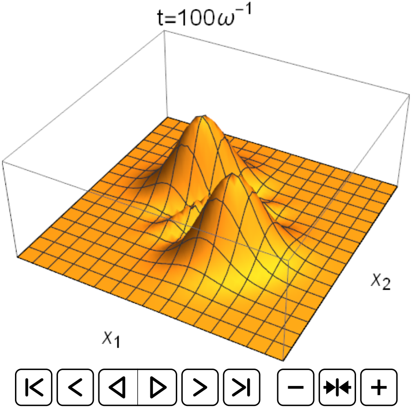
(b) - binding energies correspond to the energies of the initial "closed" trapping potential

$|\psi(x_1, x_2, t)|^2$ evolution

$g = 0$

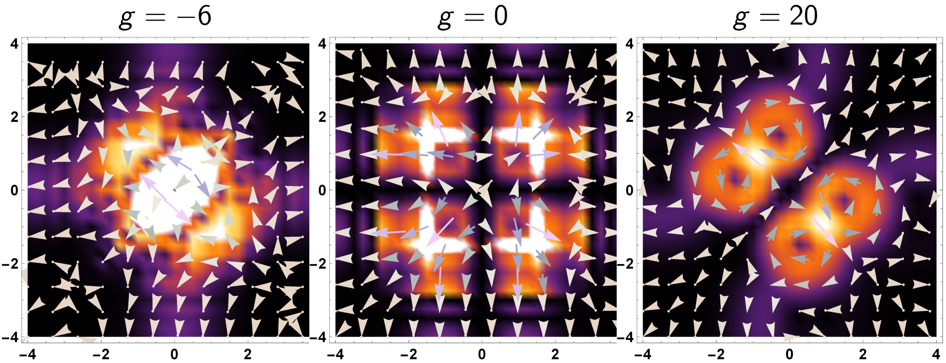


$g = -2$



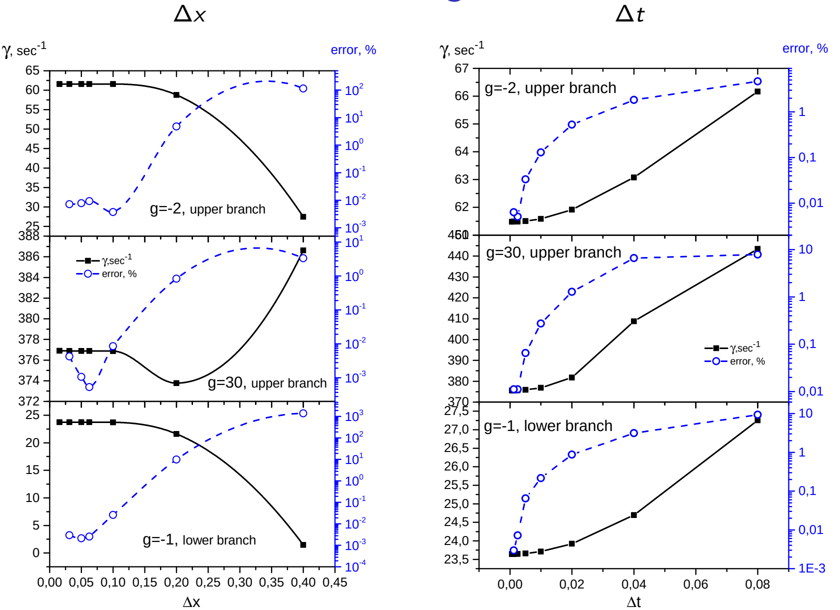
Distribution of the flux,

$$j_k(x_1, x_2) = \frac{1}{2i}\left(\psi^* \frac{\partial \psi}{\partial x_k} - \psi \frac{\partial \psi^*}{\partial x_k}\right), \quad k = 1, 2, \quad \psi(x_1, x_2)$$

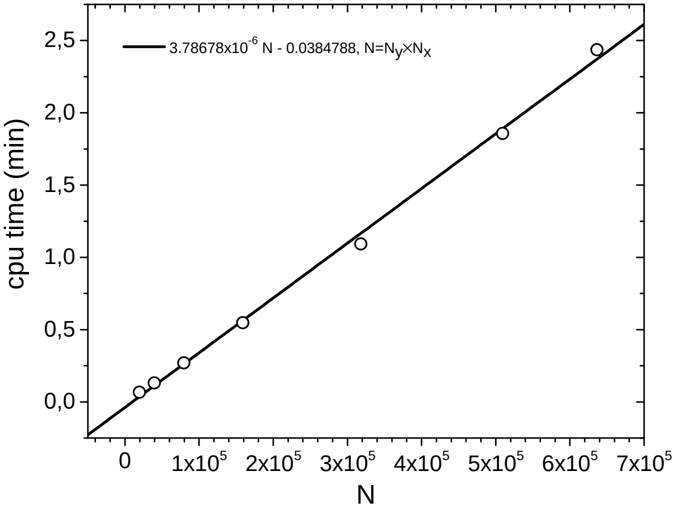


t=1msec

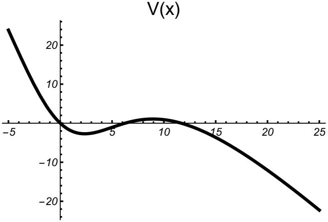
Convergence

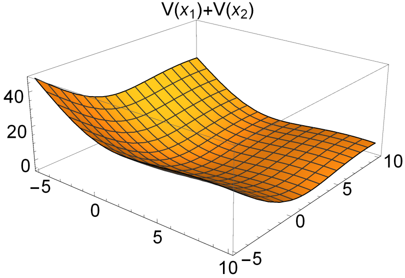


CPU time: $g = -2$


3.78678x10^-6 N - 0.0384788, N=Ny×Nx
cpu time (min)
2,5
2,0
1,5
1,0
0,5
0,0
0
1x10^5
2x10^5
3x10^5
4x10^5
5x10^5
6x10^5
7x10^5
N

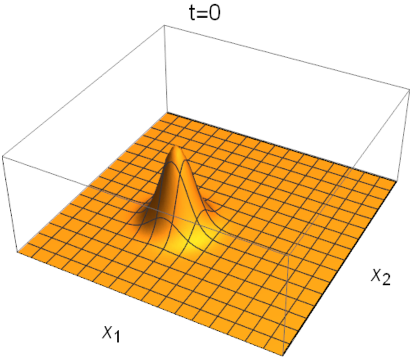
Example: S.E. Gharashi and D. Blume, (2015) *Tunneling dynamics of two interacting one-dimensional particles*, Physical Review A 92, 033629



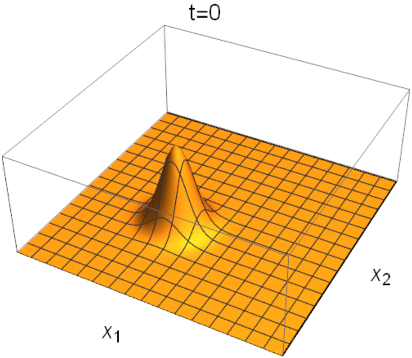


$|\psi(x_1, x_2, t)|^2$ evolution

$g = 0$



$g = -1.451$



Summary

- **efficient** computational method for the 3D time-dependent Schrödinger equation;
- **advantages** over direct methods;
- **high accuracy** confirmed for an exactly solvable 2D harmonic oscillator;
- successfully applied to a **resonant case**: a tunneling of two interacting atoms through an anharmonic barrier;
- CPU time $\sim N$
- **extension** to a more complicated problems in higher dimensions.

СПАСИБО ЗА ВНИМАНИЕ!

THANK YOU FOR YOUR ATTENTION!