Special functions and HHL Algorithm for Solving Moving Boundary Value Problems with Discontinuous Coefficients and applications in Electric Contacts

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Abstract

In this study we utilize special functions and Harrow-Hassidim-Lloyd (HHL) quantum algorithm for finding exact and approximate solutions of Generalized Heat Equation with known moving boundaries and as an example we consider model problem in spherical coordinates used for modeling electric contact erosion with Kohler's Effect. For approximate solutions of systems of MBVPs with discontinuous coefficients the collocation method was used along with the Maximum Principle for finding error estimates.

Keywords: Free Boundary Value Problems, Quantum Computing, HHL algorithm, Electric Contact Phenomena

1. Introduction

Moving Boundary Value Problems (MBVP) play impoprtant role in modeling diverse phase transitioning phenomena. Particularly different electric contact phenomena can be described using MBVPS.

Quantum computing and quantum algorithms....

Electrical contacts, their design and reliability play crucial role in designing modern electrical apparatuses. A lot of electric contact phenomena accompanied with heat and mass transfer like arcing and bridging are very rapid (nanosecond range)[1, 2] that their experimental study is very difficult or sometimes impossible and the need of their mathematical modeling is due not only

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to the need to optimize the planning experiment, but also sometimes due to the impossibility to use a different approach. Free (FBVPs) and Moving Boundary Value Problems (MBVPs) take in account phase transformations [3, 4], agree with experimental data and can serve as models for aforementioned processes [5, 6, 7].

From theoretical point of view, these problems are among the most challenging problems in the theory of non-linear parabolic equations, which along with the desired solution an unknown moving boundary has to be found. In some specific cases it is possible to construct Heat Potentials for which, boundary value problems can be reduced to integral equations [3, 4, 8]. However, in the case of domains that degenerate at the initial time, there are additional difficulties due to the singularity of integral equations, which belong to the class of pseudo - Volterra equations which can be solved in special cases and hard to solve in general case. A reader can refer to the long list of studies in [9] and literature therein dedicated to the MBVPs. Despite the great value and exhaustiveness of all these results, investigation and elaboration of both exact and approximate methods for solving MBVPs responsible for adequate modeling electric contact phenomena is still an actual mathematical problem.

In this paper we consider a class of PDEs with moving boundaries

$$\frac{\partial \theta}{\partial t} = a^2 \left(\frac{\partial \theta^2}{\partial x^2} + \frac{\nu}{x} \frac{\partial \theta}{\partial x} \right), \quad \alpha(t) < x < \beta(t), \quad -\infty < \nu < \infty, \quad t > 0, \tag{1}$$

which can be solved by the series of linear combinations of special functions which apriori satisfy equation 1

$$S^1_{\gamma,\nu}(x,t) = \left(2a\sqrt{t}\right)^\gamma \Phi\left(-\frac{\gamma}{2}, \frac{\nu+1}{2}; -\frac{x^2}{4a^2t}\right), \quad -\infty < \gamma, \nu < \infty, \tag{2}$$

$$S^2_{\gamma,\nu}(x,t) = \left(2a\sqrt{t}\right)^\gamma \left(\frac{x^2}{4a^2t}\right)^{\frac{1-\nu}{2}} \Phi\left(\frac{1-\nu-\gamma}{2}, \frac{3-\nu}{2}; -\frac{x^2}{4a^2t}\right). \tag{3}$$

Generalized Heat Equation and its solutions were studied in [10, 11, 12, 13, 14], and was successfully applied in [5, 6, 7, 15] for modeling and solving Heat and Mass transfer problems in diverse electric contact phenomena. Our goal in this series of studies is to develop new computational methods for solving MBVPs where we will be employing and developing quantum algorithms as well.

Pioneering studies [16, 17] in 1980s gave a birth to a new paradigm in computation which we call nowadays quantum computing, whereby information is encoded in a quantum system. Further on, in 1990s a series of studies [18, 19, 20] dedicated to quantum algorithms provided exponential speed-up in run time over the best known classical algorithms for same tasks. In last decades, consistent advances in theory and experiments generated a plethora of powerful quantum algorithms [21] which surpass their classical counterparts in terms of computational power, however worth noting that their applications are restricted to few use cases due to the challenges related to their physical realization. Careful physical realization may lead to profound results in reaching exponential speed-up.

In this particular study, we will be using one of such powerful quantum algorithms developed by Harrow-Hassidim-Lloyd (HHL) [22] to solve MBVPs. The HHL algorithm, its modifications and improvements [22, 23, 24, 25, 26, 27] (both for sparse and dense matrices) is the operator inversion or linear systems solving quantum algorithm, has wide range of applications [24] as well as attempts to dequantize them [28] and provides exponential speed-up over the classical algorithms. For detailed survey on improvements and limitations, complexity, QRAM and physical implementation of the algorithm we refer reader to [24, 27] and literature therein.

We consider a linear operator equation

$$Mx = b, \tag{4}$$

where in this study we assume that M is Hermitian and s-sparse matrix, and b is a vector column. This condition can be relaxed and it can be shown that $\tilde{M} = \begin{bmatrix} 0 & M \\ M^T & 0 \end{bmatrix}$ can be brought to Hermitian matrix. Since $\tilde{M}$ is Hermitian, we can solve the equation $\tilde{M}\vec{y} = \begin{bmatrix} \vec{b} \\ 0 \end{bmatrix}$ to obtain $y = \begin{bmatrix} 0 \\ \vec{x} \end{bmatrix}$. Therefore the rest of the article we assume that M is Hermitian.

The idea of the method is to reduce given MBVP to the equation 4 and apply HHL algorithm. In this study we will consider an "ideal" case where the data is encoded "efficiently" and refer reader to [27] and literature therein for different methods of Hamiltonian simulation and quantum phase estimation.

2. Main results

Let's consider the general case - the system of generalized Heat Equations with arbitrary ν, with third type boundary conditions and with known moving boundaries which can serve as a model for bridging processes in electrical contacts with variable cross section.

following formulas will ease our further calculations

$$\lim_{x\to 0}\frac{1}{z^{\beta}}\Phi\left(-\frac{\beta}{2},\mu;-z^2\right)=\frac{\Gamma(\mu)}{\Gamma(\mu+\frac{\beta}{2})}, \tag{5}$$

$$\frac{\partial\theta}{\partial x}=\sum_{n=0}^{\infty}\left(4a_1^2t\right)^n\Bigg[A_n\left(\frac{-x}{4a_1^2t}\right)L_{n-1}^{\mu}\left(\frac{-x^2}{4a_1^2t}\right)+B_n\left(\frac{x^2}{4a_1^2t}\right)^{-\mu}\left(\frac{2x}{4a_1^2t}\right)\Bigg((1-\mu)$$
$$\Phi\left(1-\mu-n,2-\mu,\frac{-x^2}{4a_1^2t}\right)-\left(\frac{-x^2}{4a_1^2t}\right)^{-\mu}\left(\frac{x^2}{4a_1^2t}\right)\Phi\left(2-\mu-n,3-\mu,\frac{-x^2}{4a_1^2t}\right)\Bigg)\Bigg], \tag{6}$$

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=\sqrt{t}}=\sum_{n=0}^{\infty}\left(4a_1^2\right)^n\left(2a_1\sqrt{t}\right)^{2n-1}\left(\frac{-\alpha}{a_1}\right)\Bigg[A_n\left(L_{n-1}^{\mu}\left(\frac{-\alpha}{2a_1}\right)\right)+B_n\Bigg((\mu-1)$$
$$\left(\frac{\alpha^2}{4a_1^2}\right)^{-\mu}\Phi\left(1-\mu-n,2-\mu,\frac{-\alpha^2}{4a_1^2}\right)+(\mu-1)\left(\frac{\alpha^2}{4a_1^2}\right)^{-\mu}\Phi\left(1-\mu-n,2-\mu,\frac{-\alpha^2}{4a_1^2}\right)\Bigg)\Bigg]. \tag{7}$$

2.1. HHL algorithm for exact solution of one phase MBVPs

$$\frac{\partial\theta}{\partial t}=a^2\left(\frac{\partial\theta^2}{\partial x^2}+\frac{\nu}{x}\frac{\partial\theta}{\partial x}\right), \qquad 0<x<\alpha\sqrt{t},\quad 0<\nu,t<1, \tag{8}$$

$$\theta(0,0)=T_m, \qquad , \tag{9}$$

$$\left.\left(\beta\theta+\gamma\frac{\partial\theta}{\partial x}\right)\right|_{x=0}=P(t), \tag{10}$$

$$\delta\theta|_{x=\alpha\sqrt{t}}=T_m, \tag{11}$$

from 2 and 3 one can obtain solutions for equations **??**,**??** and **??** in the form of following series of linear combinations of special functions

$$\theta(x,t)=\sum_{n=0}^{\infty}\left(4a^2t\right)^n\left[A_nL_n^{\mu-1}\left(\frac{-x^2}{4a^2t}\right)+B_n\left(\frac{x^2}{4a^2t}\right)^{1-\mu}\Phi\left(1-\mu-n,2-\mu,\frac{-x^2}{4a^2t}\right)\right] \tag{12}$$

Where $\mu=\frac{1+\nu}{2}$, $\beta=2n$. From conditions 10, 11 and using formula 7 we get following expressions:

$$\beta\sum_{n=0}^{\infty}\left(4a_1^2t\right)^nA_nL_n^{\mu-1}(0)=\sum_{n=0}^{\infty}P^n(0)\frac{t^n}{n!}, \tag{13}$$

$$\delta\sum_{n=0}^{\infty}\left(4a_1^2t\right)^n\left[A_nL_n^{\mu-1}\left(\frac{-\alpha^2}{4a_1^2}\right)+B_n\left(\frac{\alpha^2}{4a_1^2}\right)^{1-\mu}\Phi\left(1-\mu-n,2-\mu,\frac{-\alpha^2}{4a_1^2}\right)\right]=T_m, \tag{14}$$

After comparing coefficients at same powers of t^n, equations 13, 14 can be represented in the form of system of linear algebraic equations or in the form of matrix equation 4 or following matrix where

$$M = \begin{pmatrix} m_{11} & m_{12} & 0 & \dots & 0 & 0 & 0 \\ m_{21} & m_{22} & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ \vdots & & & \ddots & & & \vdots \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & m_{2k+12k+1} & m_{2k+12k+2} \\ 0 & 0 & 0 & \dots & 0 & m_{2k+22k+1} & m_{2k+22k+2} \end{pmatrix}, \tag{15}$$

$$x = \begin{pmatrix} A_0 \\ B_0 \\ A_1 \\ B_1 \\ \vdots \\ A_k \\ B_k \end{pmatrix}, b = \begin{pmatrix} P_0 \\ T_m \\ P_1 \\ T_m \\ \vdots \\ P_k \\ T_m \end{pmatrix},$$

where

$$\begin{aligned} m_{2k+12k+1} &= \beta \left(4a_1^2\right)^n L_n^{\mu-1}(0), \\ m_{2k+12k+2} &= 0, \\ m_{2k+22k+1} &= \delta \left(4a_1^2\right)^n L_n^{\mu-1}\left(\frac{-\alpha^2}{4a_1^2}\right) \\ m_{2k+22k+2} &= \delta \left(4a_1^2\right)^n \left(\frac{\alpha^2}{4a_1^2}\right)^{1-\mu} \Phi\left(1-\mu-n, 2-\mu, \frac{-\alpha^2}{4a_1^2}\right) \end{aligned}$$

and expressions $i^n erfc\left(\frac{\pm\alpha}{2a_j}\right)$, $i^n erfc(0)$ for $j = 1, 2,\ n = -1, 0, ..., k$ are numbers which can be determined from tables or by calculators. Next, we use algorithm 1 for solving equation 4 with entries given in formula 15 and refer reader to [29] for more details on numerical experiment in Qiskit.

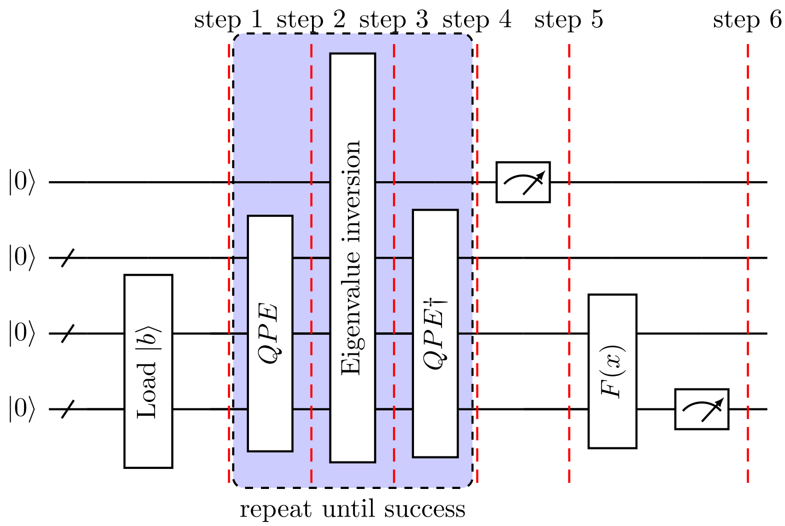

Figure 1: Quantum HHL algorithm.

2.2. HHL algorithm for exact solution of two phase MBVPs with discontinuous coefficients

Let's consider following system of generalized Heat Equations with known moving boundary and discontinuous coefficients

$$\frac{\partial \theta_1}{\partial t} = a_1^2 \left(\frac{\partial \theta_1^2}{\partial x^2} + \frac{\nu}{x} \frac{\partial \theta_1}{\partial x} \right), \qquad 0 < x < \alpha\sqrt{t}, \quad 0 < \nu, t < 1, \tag{16}$$

$$\frac{\partial \theta_2}{\partial t} = a_2^2 \left(\frac{\partial \theta_2^2}{\partial x^2} + \frac{\nu}{x} \frac{\partial \theta_2}{\partial x} \right), \qquad \alpha\sqrt{t} < x < \infty, \tag{17}$$

$$\theta_1(0,0) = T_m, \tag{18}$$

$$\theta_2(x,0) = f(x), \tag{19}$$

$$f(0) = T_m,\ \alpha(0) = 0, \qquad \lim_{x\to\infty} f(x) \approx f(X) = 0, \quad , \tag{20}$$

$$\left(\beta\theta_1 + \gamma \frac{\partial \theta_1}{\partial x} \right)\Big|_{x=0} = P(t), \tag{21}$$

$$\delta\theta_1|_{x=\alpha\sqrt{t}} = \kappa\theta_2|_{x=\alpha\sqrt{t}} = T_m \tag{22}$$

The solution of problem 16-22 can be represented in the following form

$$\theta_1(x,t) = \sum_{n=0}^{\infty} \left(4a_1^2 t\right)^n \left[A_n L_n^{\mu-1}\left(\frac{-x^2}{4a_1^2 t}\right) + B_n \left(\frac{x^2}{4a_1^2 t}\right)^{1-\mu} \Phi\left(1-\mu-n, 2-\mu, \frac{-x^2}{4a_1^2 t}\right)\right] \tag{23}$$

$$\theta_2(x,t) = \sum_{n=0}^{\infty} \left(4a_2^2 t\right)^n \left[C_n L_n^{\mu-1}\left(\frac{-x^2}{4a_2^2 t}\right) + D_n \left(\frac{x^2}{4a_2^2 t}\right)^{1-\mu} \Phi\left(1-\mu-n, 2-\mu, \frac{-x^2}{4a_2^2 t}\right)\right] \tag{24}$$

From 21,22,19,5,7, we get

$$\beta \sum_{n=0}^{\infty} \left(4a_1^2 t\right)^n A_n L_n^{\mu-1}(0) = \sum_{n=0}^{\infty} P^n(0)\frac{t^n}{n!}, \tag{25}$$

$$\delta \sum_{n=0}^{\infty} \left(4a_1^2 t\right)^n \left[A_n L_n^{\mu-1}\left(\frac{-\alpha^2}{4a_1^2}\right) + B_n \left(\frac{\alpha^2}{4a_1^2}\right)^{1-\mu} \Phi\left(1-\mu-n, 2-\mu, \frac{-\alpha^2}{4a_1^2}\right)\right] = T_m, \tag{26}$$

$$\frac{(-1)^n}{n!} C_n + D_n = \frac{f^{2n}(0)}{(2n)!}, \tag{27}$$

$$\kappa \sum_{n=0}^{\infty} \left(4a_2^2 t\right)^n \left[C_n L_n^{\mu-1}\left(\frac{-\alpha^2}{4a_2^2}\right) + D_n \left(\frac{\alpha^2}{4a_2^2}\right)^{1-\mu} \Phi\left(1-\mu-n, 2-\mu, \frac{-\alpha^2}{4a_2^2}\right)\right] = T_m. \tag{28}$$

Let $P(t) = \sum_{n=0}^{k} P_n t^n$, where $P_n = \frac{P^n(0)}{n!}$ and have to be determined from boundary and initial conditions. The idea of the collocation method applied in this problem is to subdivide $0 < t < T_a$ into k intervals and after substituting solution functions **??**, **??** into the boundary conditions **??**,**??**,**??** at points $t_1, t_2, ..., t_k$ solve the system of linear algebraic equation or matrix equation 4 for coefficients A_n, B_n, C_n, P_n using HHL algorithm, where M, x, b in equation 4 are as following:

$$M = \begin{pmatrix} m_{11} & m_{12} & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ m_{21} & m_{22} & 0 & 0 & \dots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & m_{33} & m_{34} & \dots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & m_{43} & m_{44} & \dots & 0 & 0 & 0 & 0 & 0 \\ \vdots & & & & \ddots & & & & & \vdots \\ 0 & 0 & 0 & 0 & \dots & 0 & m_{4k-3,4k-3} & m_{4k-3,4k-2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & m_{4k-2,4k-3} & m_{4k-2,4k-2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & m_{4k-1,4k-1} & m_{4k-1,4k} \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & 0 & m_{4k,4k-1} & m_{4k,4k} \end{pmatrix}, \tag{29}$$

$$x = \begin{pmatrix} A_0 \\ B_0 \\ C_0 \\ D_0 \\ \vdots \\ A_k \\ B_k \\ C_k \\ D_k \end{pmatrix}, b = \begin{pmatrix} P_0 \\ T_m \\ \frac{f^{(0)}(0)}{(0)!} \\ T_m \\ \vdots \\ P_k \\ T_m \\ \frac{f^{(2n)}(0)}{(2n)!} \\ T_m \end{pmatrix},$$

where

$$
\begin{aligned}
m_{4k-3,4k-3} &= \beta \left(4a_1^2\right)^n L_n^{\mu-1}\left(0\right), \\
m_{4k-3,4k-2} &= 0, \\
m_{4k-2,4k-3} &= \delta \left(4a_1^2\right)^n L_n^{\mu-1}\left(\frac{-\alpha^2}{4a_1^2}\right) \\
m_{4k-2,4k-2} &= \delta \left(4a_1^2\right)^n \left(\frac{\alpha^2}{4a_1^2}\right)^{1-\mu} \Phi\left(1-\mu-n, 2-\mu, \frac{-\alpha^2}{4a_1^2}\right) \\
m_{4k-1,4k-1} &= \frac{(-1)^n}{(n)!}, \\
m_{4k-1,4k} &= \frac{(-1)^n}{(n)!}, \\
m_{4k,4k-1} &= \kappa \left(4a_2^2\right)^n L_n^{\mu-1}\left(\frac{-\alpha^2}{4a_2^2}\right) \\
m_{4k,4k} &= \kappa \left(4a_2^2\right)^n \left(\frac{\alpha^2}{4a_2^2}\right)^{1-\mu} \Phi\left(1-\mu-n, 2-\mu, \frac{-\alpha^2}{4a_2^2}\right)
\end{aligned}
$$

Next, we use Quantum HHL algorithm 1 for solving problem 4 with entries given in **??**. Numerical implementation is demonstrated in [29].

Algorithm 1: Quantum HHL Algorithm in Qiskit

Data: Load the data $|b\rangle \in \mathbb{C}^N$

Result: Apply an observable M to calculate $F(x) = \langle x| M |x\rangle$.

initialization;

while *outcome is not* 1 **do**

- Apply Quantum Phase Estimation (QPE) with $U = e^{iMt} := \sum_{j=0}^{N-1} e^{i\lambda_j t} |u_j\rangle \langle u_j|$. Which implies $\sum_{j=0}^{N-1} b_j |\lambda_j\rangle_{n_l} \langle u_j|_{n_b}$, in the eigenbasis of M where $|\lambda_j\rangle_{n_l}$ is the n_l -bit binary representation of λ_j .
- Add an ancilla qubit and apply a rotation conditioned on $|\lambda_j\rangle$, $\sum_{j=0}^{N-1} b_j |\lambda_j\rangle_{n_l} \langle u_j|_{n_b} \left(\sqrt{1 - \frac{C^2}{\lambda_j^2}} |0\rangle + \frac{C}{\lambda_j} |1\rangle\right)$, C - normalization constant.
- Apply $QPE^{\dagger}$. This results in $\sum_{j=0}^{N-1} b_j |0\rangle_{n_l} \langle u_j|_{n_b} \left(\sqrt{1 - \frac{C^2}{\lambda_j^2}} |0\rangle + \frac{C}{\lambda_j} |1\rangle\right)$;

if *If the outcome is* 1 *, the register is in the post-measurement state* $\left(\sqrt{\frac{1}{\sum_{j=1}^{N-1} |b_j|^2/|\lambda_j|^2/}}\right) \sum_{j=0}^{N-1} \frac{b_j}{\lambda_j} |0\rangle_{n_l} \langle u_j|_{n_b}$ **then**

Apply an observable M to calculate $F(x) = \langle x| M |x\rangle$;

else

repeat the loop;

end

end

For computational purposes we use Qiskit and IBM Q. Let's consider exact and approximate solutions of two model problems where we demonstrate the use of HHL quantum algorithm. The error of the approximate solution can be estimated by the Maximum Principle.

3. Experimental Results and Discussion

3.1. Experimental Results on IBM Quantum with Qiskit

We used IBM Q and Qiskit for experiments and programming purposes. MBVP and the Inverse Two-Phase Stefan Problem were solved with fidelities 0.99 and 1 respectively. We refer reader to

[29] for details of experiments. Proposed method in combination with Fa Di Bruno's Formula and Quantum HHL algorithm can be used for exact solutions for direct/inverse Stefan type problems and MBVPs in general for arbitrary ν in 1 and arbitrary $\alpha(t)$. Special functions method in combination with HHL algorithm or its Continuous Variable version [32] can be also used for approximate solutions of boundary value problems with fixed boundaries as well.

4. Conclusion

Special functions method and HHL quantum algorithm was used for exact solutions of one and two moving boundary value problems. We used IBM Q for experiments [29] and solved MBVP with discontinuous coefficients. $A_0, A_1, B_0, B_1, C_0, C_1$ coefficients of solution functions in **??**,**??** and **??**,**??** were found with fidelities 0.99 and 1 respectively.

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