Special Functions and HHL Quantum Algorithm for Solving Moving Boundary Value Problems Occurring in Electric Contact Phenomena

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Abstract—This series of studies is devoted to developing and employing mathematical methods along with quantum algorithms for solving moving boundary value problems which occur in heat and mass transfer problems. In this particular study we develop mathematical framework where we utilize special functions and Harrow-Hassidim-Lloyd (HHL) quantum algorithm for finding exact and approximate solutions of Generalized Heat Equation with moving boundaries and as examples we consider plane and spherical cases. In spherical case the Generalized Heat Equation is reduced to linear moving boundary value problem with discontinuous coefficients and solved exactly. In plane case we use collocation method for approximate solution of Inverse Two-Phase Stefan problem. Experimental verification of suggested mathematical framework has been tested for modeling arcing phenomena in composite electrical contacts with AgCdO (90%) and Ni (10%). HHL algorithm was applied and run on IBM Q with Qiskit and the code is openly available on https://github.com/users/Schrodinger-cat-kz/projects/2.

Index Terms—electric contacts, HHL algorithm, special functions, Stefan problem, moving and free boundary value problems

I. INTRODUCTION

Free and moving boundary value 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 [1]–[3]. 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 [4] 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 heat and mass transfer problems particularly in electric contact phenomena is still an actual mathematical problem, which we will be considering in this series of studies. In this paper we consider a class of PDEs with moving boundaries

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

$$-\infty < \nu < \infty, \quad t > 0,$$

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

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

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

where \( \Phi \) is a hypergeometric function. Generalized Heat Equation and its solutions were studied in [5]–[9], and were successfully applied in [10]–[13] 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 [14], [15] 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 [16]–[18] 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 [19] 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) [20] to solve MBVPs. The HHL algorithm, its modifications and improvements [20]–[25] (both for sparse and dense matrices) is the operator inversion or linear systems solving quantum algorithm, has wide range of applications [22] as well as attempts to dequantize them [26] 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 [22], [25] and literature therein.

We consider a linear operator equation

\[ M |x\rangle = |b\rangle, \quad (4) \]

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 e.d. if \( M \) is not Hermitian and it can be shown that \( \hat{M} = \begin{bmatrix} 0 & M^T \\ M & 0 \end{bmatrix} \) can be brought to Hermitian matrix. Since \( \hat{M} \) is Hermitian, we can solve the equation \( \hat{M} |\tilde{y}\rangle = |\tilde{b}\rangle \) to obtain \( |y\rangle = \begin{bmatrix} 0 \\ x \end{bmatrix} \). 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 [25] and literature therein for different methods of Hamiltonian simulation and quantum phase estimation.

II. MAIN RESULTS

Equation (1) with arbitrary \( \nu \) is a generalized heat equation which can serve as a model for bridging processes in electrical contacts with variable cross section. For \( \nu = 0, 1, 2 \) equation (1) is transformed to the following heat equations in linear, spherical and cylindrical coordinates respectively

\[ \frac{\partial \theta}{\partial t} = a^2 \frac{\partial^2 \theta}{\partial x^2}, \quad \alpha(t) < x < \beta(t), t > 0 \]

\[ \frac{\partial \theta}{\partial t} = a^2 \left( \frac{\partial^2 \theta}{\partial x^2} + \frac{1}{x} \frac{\partial \theta}{\partial x} \right), \quad \alpha(t) < x < \beta(t), t > 0 \]

\[ \frac{\partial \theta}{\partial t} = a^2 \left( \frac{\partial^2 \theta}{\partial z^2} + \frac{2}{x} \frac{\partial \theta}{\partial x} \right), \quad \alpha(t) < x < \beta(t), t > 0 \]

and from (2) and (3) one can obtain solutions for equations (5),(6) and (7) in the form of following series of linear combinations of special functions

\[ \theta(x, t) = \sum_{n=0}^{k} \left( 2a^2 \mu \right)^n \left[ a_n i^n \text{erfc} \left( \frac{x}{2a^2 \mu} \right) + \right. \]

\[ B_n i^n \text{erfc} \left( -\frac{x}{2a^2 \mu} \right) \]

\[ \theta(x, t) = \sum_{n=0}^{k} F_n \frac{n!}{(2n)!} \left( 4a^2 t \right)^n L_n \left( -\frac{x}{4a^2 t} \right), \]

\[ \theta(x, t) = \frac{1}{x} \sum_{n=0}^{k} \left( 2a^2 \mu \right)^n \left[ C_n i^n \text{erfc} \left( \frac{x}{2a^2 \mu} \right) + \right. \]

\[ D_n i^n \text{erfc} \left( -\frac{x}{2a^2 \mu} \right), \]

where coefficients \( A_n, B_n, C_n, D_n, F_n \) and \( k \) have to be determined and can be found from boundary and initial conditions subject to corresponding equations (5),(6) and (7) by using quantum HHL algorithm. After substituting solution functions into boundary conditions, the problem is reduced to the system of linear algebraic equations which are solved by the HHL algorithm. As for arbitrary moving boundary \( \alpha(t) \) coefficients of solution functions are calculated in the same manner in combination with Faa Di Bruno’s formula and HHL Algorithm. Following formula is useful for determining coefficients in (8), (9) and (10) from initial conditions of corresponding MBVPs considered in following sections

\[ \lim_{x \rightarrow 0} \frac{1}{z^\beta} \frac{\Phi \left( -\frac{\beta}{2}, \mu; -z^2 \right)}{\Gamma \left( \mu + \frac{\beta}{2} \right)} = \frac{\Gamma(\mu)}{\Gamma(\mu + \frac{\beta}{2})}. \]

Exact or approximate solutions of (1) for arbitrary \( \nu \) can be reduced to system of linear algebraic equations or (4). The HHL algorithm applied for solving MBVPs provides exponential speedup run time over the classical algorithm under the ideal case assumption i.e. Hamiltonian simulation, phase estimation, load and read out of data are implemented "efficiently".

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.

A. HHL algorithm for exact solution of system of MBVP with discontinuous coefficients

For electric contacts with small contact surface area (with contact radius \( b < 10^{-4} \) m.) and low electric current, Holm’s ideal sphere [30] and following system of spherical heat equations \( (\nu = 2 \text{ in } (1)) \) can be sufficient for adequate modeling and investigation of diverse electric contact phenomena for example heat transfer in closed electric contacts where \( \theta_1 \)
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 $U = e^{iM\hat{H}} = \sum_{j=0}^{N-1} e^{i\lambda_j t} |u_j\rangle\langle u_j|$ where $\lambda_j\langle n_l |$ is the $n_l$-bit binary representation of $\lambda_j$.
- Add an ancilla qubit and apply a rotation conditioned on $|\lambda_j\rangle$,
  $$\sum_{j=0}^{N-1} b_j |\lambda_j\rangle_{n_l} \langle u_j|_{n_b} \left( \sqrt{1 - \frac{C^2}{\lambda_j^2}} |0\rangle + \frac{C}{\lambda_j} |1\rangle \right),$$
- Apply QPE$'$.

if the outcome is 1, the register is in the post-measurement state

$$\left( \frac{1}{\sqrt{\sum_{j=0}^{N-1} |b_j|^2}} \right) \sum_{j=0}^{N-1} b_j |\lambda_j\rangle_{n_l} \langle u_j|_{n_b}$$

- Apply an observable $M$ to calculate $F(x) = \langle x | M | x \rangle$;
else repeat the loop;
end

$T_m$ is the melting temperature at moving boundary. For the sake of simplicity we omit Stefan condition and consider $\alpha\sqrt{t}$ ($\alpha$-const.) - known, moving boundary function which is a good approximation and widely used in applied problems. Let’s consider following MBVP:

$$\frac{\partial U_1}{\partial t} = a_1^2 \frac{\partial^2 U_1}{\partial x^2}, \quad 0 < x < \alpha\sqrt{t}, t > 0,$$
$$\frac{\partial U_2}{\partial t} = a_2^2 \frac{\partial^2 U_2}{\partial x^2}, \quad \alpha\sqrt{t} < x < \infty, t > 0,$$
$$U_1(0,0) = 0,$$
$$U_2(x,0) = f(x),$$
$$\sigma \frac{\partial U_1}{\partial x} \bigg|_{x=\alpha\sqrt{t}} = \frac{\partial U_1}{\partial x} \bigg|_{x=\alpha\sqrt{t}},$$
$$U_1(\alpha\sqrt{t}, t) = U_2(\alpha\sqrt{t}, t)$$
$$U_2(\infty, 0) = 0.$$

We represent exact solution in the form of series

$$U_1(x,t) = \sum_{n=0}^{k} \left( 2a_1 \sqrt{t} \right)^n \left[ A_n t^n \operatorname{erfc} \left( \frac{x}{2a_1 \sqrt{t}} \right) \right],$$
$$U_2(x,t) = \sum_{n=0}^{k} \left( 2a_2 \sqrt{t} \right)^n \left[ C_n t^n \operatorname{erfc} \left( \frac{x}{2a_2 \sqrt{t}} \right) \right],$$

where $k$, $A_n$, $B_n$, $C_n$, $D_n$ are defined from initial and boundary conditions. The problem is reduced to the problem (4) and solved using HHL algorithm. Computational details are demonstrated in our public github repository [29].

B. HHL algorithm for approximate solution of the Inverse Two-Phase Stefan Problem

In previous section we considered $\alpha\sqrt{t}$ case, for arbitrary $\alpha(t)$ boundary we follow the same principle and can use Fa Di Bruno’s Formula in combination with HHL quantum algorithm to find exact solutions. However, worth noting that, in electrical engineering, it’s sometimes sufficient and useful to utilize approximate solutions of the problems where error can be estimated using the Maximum principle. In this section we will demonstrate the use of HHL algorithm for approximate solution (collocation method) of the Inverse Two-Phase Stefan Problem which is used for modeling arcing processes and determining heat flux function [27].
Stefan problem is a type of free boundary value problems where along with a temperature function \( \theta \) in (12) and (13), an unknown moving boundary has to be determined. In inverse Stefan problems moving boundary is given and known, the goal is to reconstruct functions at boundary conditions and temperature functions in system of Heat Equations. These problems are widely used for modeling wide range of transient phenomena in chemistry, physics, biology and economics [4], [28]. In the problem below, moving boundary \( \alpha(t) \) is given and besides temperature function \( \theta \) in (24),(25), flux function \( P(t) \) has to be determined. Let’s consider following linear Inverse Two-Phase Stefan Problem

\[
\frac{\partial \theta_1}{\partial t} = a_1^2 \frac{\partial^2 \theta_1}{\partial x^2}, \quad 0 < x < \alpha(t), 0 < t < t_a
\]  

(24)

\[
\frac{\partial \theta_2}{\partial t} = a_2^2 \frac{\partial^2 \theta_2}{\partial x^2}, \quad \alpha(t) < x < X, 0 < t < t_a
\]  

(25)

\[
\theta_1(0,0) = T_m,
\]  

(26)

\[
\theta_2(x,0) = f(x),
\]  

(27)

\[
f(0) = T_m, \alpha(0) = 0, \lim_{x \to \infty} f(x) = f(X) = 0,
\]  

\[
\lim_{x \to \infty} \theta(x,t) \approx \theta(X,t) = 0,
\]  

(28)

\[
- \lambda_1 \frac{\partial \theta_1}{\partial x} \bigg|_{x=0} = P(t),
\]  

(29)

\[
\theta_1(\alpha(t),t) = \theta_2(\alpha(t),t) = T_m
\]  

(30)

\[
- \lambda_1 \frac{\partial \theta_1}{\partial x} \bigg|_{x=\alpha(t)} = - \lambda_2 \frac{\partial \theta_2}{\partial x} \bigg|_{x=\alpha(t)} + L \gamma \frac{\partial \alpha(t)}{\partial t}
\]  

(31)

where \( T_m, X \) and \( t_a \) are melting temperature, finite electric contact radius and arcing duration respectively.

Following analogy in section II-A we represent solution in the form of series

\[
U_1(x,t) = T_m + \sum_{n=0}^{k} \left( \frac{2a_1 \sqrt{t}}{n} \right)^n A_n,
\]  

(32)

\[
i^n erfc \left( \frac{x}{2a_1 \sqrt{t}} \right) + B_n i^n erfc \left( \frac{-x}{2a_1 \sqrt{t}} \right),
\]  

\[
U_2(x,t) = T_m + \sum_{n=0}^{k} \left( \frac{2a_2 \sqrt{t}}{n} \right)^n C_n,
\]  

(33)

\[
i^n erfc \left( \frac{x}{2a_2 \sqrt{t}} \right) + D_n i^n erfc \left( \frac{-x}{2a_2 \sqrt{t}} \right),
\]  

where coefficients \( D_n \) at (33) can be found from (27) exactly. Thus

\[
D_n = \frac{f^n(0)}{2}.
\]  

(34)

Let \( P(t) = \sum_{n=0}^{k} P_n t^n \), where \( P_n = \frac{\rho_n}{\rho_1} \) 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 (32), (33) into the boundary conditions (29),(30),(31) at points \( t_1, t_2, \ldots, t_k \) reduce the problem to the equation (4) and solve for coefficients \( A_n, B_n, C_n, P_n \) using HHL algorithm. We refer the reader to our public github repository [29] for more computational details.

III. EXPERIMENTAL RESULTS AND DISCUSSION

In this section we show that suggested framework can be used for modeling and solving heat and mass transfer problems occurring in arc erosion of opening composite electrical contacts (AgCdO 90%, Ni 10%). We also show that aforementioned heat and mass transfer problems can be solved using combination of special functions and HHL algorithm. For computational purposes we use Qiskit on IBM Q and refer reader to [29] for details of the code which is publicly open.

A. Experimental verification of mathematical model

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) [30], [31] that their experimental study is very difficult or sometimes impossible and the need of their mathematical modeling is due not only 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 [1], [2], agree with experimental data and can serve as models for aforementioned processes [10]–[12].

We use direct two-phase spherical Stefan problem for modeling arcing process in opening AgCdO contacts in air at 1 atmosphere pressure and Ni contacts in a chamber at varied pressure. Electrical circuit diagram of the test rig is presented in Fig. 2

![Fig. 2. Electric circuit](image)

The values of measured parameters for both contact materials are given in the Table

The corresponding arc power \( P_A(t) \) for this electrical circuit is calculated in the paper [32] and presented for
If we identify the arc radius $r_a$ with the initial radius of melting isotherm $\alpha(0) = b$, then the heat flux $P(t)$ in the condition (29) can be defined as $P(t) = P_A(t)/\pi r_a^2$.

The thermophysical parameters for AgCdO (Ag-90%, CdO-10%) are following [33]:

$$T_m = 1233 \text{ K}, \quad \gamma = 10.21 \cdot 10^3 \text{ kg} \cdot \text{m}^{-3},$$
$$L = 1.06 \cdot 10^9 \text{ J} \cdot \text{m}^{-3}, \quad \lambda_1 = 307 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1},$$
$$\lambda_2 = 285 \text{ W} \cdot \text{m}^{-1} \cdot \text{K}^{-1}, \quad a_1 = 0.011 \text{ W} \cdot \text{m} \cdot \text{sec}^{-1/2},$$
$$a_2 = 0.008 \text{ W} \cdot \text{m} \cdot \text{sec}^{-1/2},$$

The initial temperature $f(r)$ can be determined from the expression for the temperature at the pre-melting stage at the time $t_m$, when its value on the boundary $r = b$ reaches the melting point:

$$f(r) = \frac{a_2 b}{\lambda_2 r} \int_0^{t_m} \left[ \frac{\exp \left( \frac{(r-b)^2}{4a_2^2(t_m-\tau)} \right)}{\sqrt{\pi(t_m-\tau)}} - \frac{a_2}{b} \right] \exp \left( \frac{1}{b} (r-b) + \frac{a_2^2}{b^2} (t_m - \tau) \right) \text{erfc} \left( \frac{r-b}{2a_2 \sqrt{(t_m-\tau)}} \right) P(\tau) d\tau. \quad (35)$$

where $t_m$ should be defined from the equation:

$$T_m = \frac{a_2}{\lambda_2} \int_0^{t_m} \left[ \frac{1}{\sqrt{\pi(t_m-\tau)}} - \frac{a_2}{b} \right] \exp \left( \frac{a_2^2}{b^2} (t_m - \tau) \right) \text{erfc} \left( \frac{a_2}{b} \sqrt{(t_m-\tau)} \right) P(\tau) d\tau \quad (36)$$

The results of calculation of the temperature distribution on the contact spot are $t_m = 0.4 \mu$sec, $t_b = 2.4 \mu$sec, $t_a = 7.3 \mu$sec, where $t_m$ is the time of the beginning of melting and $t_b$ is the boiling start.

One can see that the duration of the contact erosion due to boiling and evaporation is $t_0 = t_a - t_b = 4.9 \mu$sec. The mass of the evaporated sphere whose volume is $V = \frac{4}{3} \pi a^3(t_0)$ is 42.6 $\mu$g. According to the experimental data the measured erosion is 38.4 $\mu$g. This discrepancy can be explained by the fact that the presented model does not take into account the portion of the heat flux consumed for the phase transformation at boiling and operates with an overestimated flux.

**B. HHL algorithm on IBM Q with Qiskit**

We used IBM Q and Qiskit for experiments and programming purposes. $A_0, A_1, B_0, B_1, C_0, C_1$ and $A_0, A_1, B_0, B_1, C_0, C_1, F_0, P_3$ coefficients of solution functions and flux function in (22),(23) and (32),(33) of MBVP with discontinuous coefficients and the Inverse Two-Phase Stefan Problem were found with fidelities 0.99 and 1 respectively. We refer reader to [29] for details of experiments.

**IV. CONCLUSIONS**

In this study we demonstrated that suggested mathematical framework can be used for modeling and solving heat and mass transfer problems occurring in electric contacts using special functions and HHL algorithm. Proposed method in combination with Arbogast (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 $\nu$ in (1) and arbitrary $\alpha(t)$. Special functions method in combination with HHL algorithm or its Continuous Variable version [34] can be also used for approximate solutions of boundary value problems with fixed boundaries as well.

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