Detection of energy levels of a spin system on a quantum computer by probe spin evolution

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Abstract We propose a method for detection of energy levels of arbitrary spin system on a quantum computer based on studies of evolution of only one probe spin. On the basis of the proposed method energy levels of spin systems are found on IBM’s quantum computer ibmq-bogota, among them are spin chain in magnetic field, triangle spin cluster, Ising model on squared lattice, a spin in magnetic field. The results of quantum calculations are in agreement with the theoretical ones. The method is efficient for estimation of the energy levels of many-spin systems and opens a possibility to achieve quantum supremacy in solving eigenvalue problem with development of multi-qubit quantum computers.

1 Introduction

Studying of energy levels of physical systems is one of the central problems of quantum mechanics that can be solved on a quantum computer. To estimate the energies of a quantum system the quantum phase estimation algorithm was developed [1–4]. The algorithm has been widely used (see, for instance, [2–10] and references therein). For detecting of energies of transitions the robust phase estimation algorithm was introduced in [9].

Method for estimation of energy levels by time dependence of expectation values of the evolution operator was proposed [11,12]. The method is based on quantum algorithm with controlled operator of evolution (see [11]). The spectroscopy protocol to extract many-body spectra in experimental simulations was introduced in [13]. The protocol diabatically ramps the transverse magnetic field to create excitations. In [14] quantum Lanczos and quantum imaginary time evolution algorithms were proposed. Qubit efficient scheme to study ground-state properties of quantum many-body systems was suggested in [15]. Well-known method allowing to find transition energies is classical-quantum algorithm variational quantum eigensolver [16–19]. Also the ground state and therefore the energy of the state can be found with quantum approximate optimization algorithm [20–23].

In our recent paper [24] we proposed a method for detecting of the energy levels of a quantum system on a quantum computer based on studies of evolution of mean value of operator anticommuting with Hamiltonian of the system. The method was realized for detection of the energy levels of spin systems with energy levels symmetric with respect to $E \rightarrow -E$ (spin in magnetic field, spin chain, Ising model on squared lattice) on IBM’s quantum computers [24]. It is worth noting that existence of operator anticommuting with Hamiltonian is the evidence of symmetry of its energy levels with respect to $E \rightarrow -E$. Not for arbitrary Hamiltonian one can find the anticommuting operator. In the present paper we propose an efficient method for detecting of energy levels of arbitrary spin systems on a quantum computer. The method is based on studies of evolution of probe spin. We realized the method for examination of the energy levels of a spin chain in the magnetic field, triangle spin cluster, Ising model on squared lattice in the magnetic field, a spin in the magnetic field. The results of calculations of the energy levels of the spin systems on IBM’s quantum computer correspond to analytical ones.

The paper is organized as follows. In Sect. 2 the method for detecting of the energy levels of a quantum system on the basis of studies of evolution of probe spin is presented. As an example, on the basis of the proposed method we study the energy levels of spin systems described by the Ising model. Results of quantum calculations of the energy levels of spin systems on ibmq-bogota are presented in Sect. 3. Conclusions are done in Sect. 4.
2 Evolution of mean value of a probe spin and energy levels of a spin system

We study eigenvalue problem for Hamiltonian $H$

$$H|\psi\rangle = E|\psi\rangle.$$  

(1)

Energy levels are restricted from the bottom. Therefore we can shift them to the positive ones by adding constant $C$ to $H$.

Let us add to system under consideration additional spin (ancilla qubit) and construct total Hamiltonian in the following form

$$H_T = \sigma_0^x (H + C).$$  

(2)

Note that $[\sigma_0^x, H] = 0$. Eigenvalues of operator $\sigma_0^x$ are $\pm 1$. Therefore the energy spectrum of the total Hamiltonian $H_T$ contains positive eigenvalues of $H + C$ and eigenvalues of $-(H + C)$ that are negative. Note that the energy spectrum of $H_T$ is symmetric with respect to $E_T \rightarrow -E_T$ (here $E_T$ are the energy levels of $H_T$). It is easy to write operators anticommuting with the total Hamiltonian. We have

$$[\sigma_0^y, H_T] = [\sigma_0^y, H_T] = 0.$$  

(3)

Now, knowing the operator that anticommutes with Hamiltonian we can detect the energy levels corresponding to $H_T$ on the basis of studies of evolution of mean value of the operator on a quantum devise [24]. In our paper [24] it was shown that the Fourier transformation of the time dependence of the mean value has sharp peaks corresponding to double eigenvalues of the Hamiltonian.

As an example let us consider $N$ spins described by the Ising model and study its energy levels. The Hamiltonian reads

$$H = \frac{1}{2} \sum_{i,j} J_{ij} \sigma_i^z \sigma_j^z,$$  

(4)

where $J_{ij}$ represents interaction between spins.

The total system with additional spin is represented by the following Hamiltonian

$$H_T = \sigma_0^x (H + C) = \frac{1}{2} \sum_{i,j} J_{ij} \sigma_0^x \sigma_i^z \sigma_j^z + C \sigma_0^z,$$  

(5)

where constant $C$ is added to shift the energy spectrum of the Hamiltonian of a system $H$ to the positive values.

Let us consider evolution of state vector governed by $H_T$. As an initial state we choose

$$|\psi_0\rangle = |+ + \cdots +\rangle = H^{[N+1]}|00\ldots0\rangle = \frac{1}{2^{N/2}} \sum_{x_0, x_1, x_2, \ldots, x_N} |x_0 x_1 x_2 \ldots x_N\rangle,$$  

(6)

where $H^{[N+1]} = \prod_{i=0}^{N} H_i$. $H_i$ is the Hadamard operator acting on $i$-th qubit, and $x_i = 0, 1$. Qubit is associated with spin, namely, $|0\rangle = |\uparrow\rangle$ and $|0\rangle = |\downarrow\rangle$.

The evolution of the mean value of $\sigma_0^x$ reads

$$\langle \sigma_0^x(t) \rangle = \langle + + \cdots + | \sigma_0^x e^{-i2H_T t/\hbar} | + + \cdots + \rangle = \frac{1}{2^{N+1}} \sum_{x_0, x_1, x_2, \ldots, x_N} \langle x_0 x_1 x_2 \ldots x_N | e^{-i2H_T t/\hbar} | x_0 x_1 x_2 \ldots x_N \rangle = \frac{1}{2^{N+1}} \sum_{k=0}^{2^{N+1}} e^{-i2\omega_k t}.$$  

(7)

Here we take into account that $\sigma_0^x |+\rangle = |+\rangle$, $|x_0 x_1 x_2 \ldots x_N\rangle$ are the eigenstates of the total hamiltonian $H_T$, and $\omega_k$ are the energy levels in the units of $\hbar$. To extract the frequencies $\omega_k$ we consider the Fourier transformation

$$\sigma_0^x(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dt \langle \sigma_0^x(t) \rangle e^{i\omega t} = \frac{1}{2^{N+1}} \sum_i \delta (\omega - 2\omega_k).$$  

(8)

Thus function $\sigma_0^x(\omega)$ has $\delta$-peaks at $\omega = 2\omega_k$. It allows us to find the frequencies $\omega_k$ that correspond to energy levels $E_i = 2\hbar\omega_k$ of the total Hamiltonian. Positive part of this spectrum corresponds to the energy levels of the Hamiltonian of the system $H$ (4) shifted on the constant $C$.

Quantum protocol for studies of evolution of mean value of a probe spin is presented on Fig. 1. In the protocol $\alpha = 2t/\hbar$, $U(\alpha) = \exp (-i\alpha \sigma_0^x H/2)$. To quantify the mean value of $\sigma_0^x$ we take into account that the operator $\sigma_0^x$ can be represented as $\sigma_0^x = \exp(-i\pi \alpha \sigma_0^x/4) \sigma_0^x \exp(i\pi \sigma_0^x/4)$. Therefore before measurement in the standard basis the state of the corresponding qubit is rotated with $RY(-\pi/2)$ gate.

On a quantum computer we can detect values of $\langle \sigma_0^x(t) \rangle$ at fixed moments of time (fixed parameter $\alpha$). So, we have to choose the time interval $\tau$ and realize quantum protocol Fig. 1 for $\alpha = 2\tau n/\hbar$, that corresponds to $t = \tau n$, $n = -N, -N + 1, \ldots N - 1, N$. 

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In this case the total Hamiltonian (2) reads

\[ H = \sigma_1^x \sigma_2^x + J \sigma_2^y \sigma_3^y + J \sigma_1^z + J \sigma_2^z + J \sigma_3^z. \]

Let us consider a spin chain in magnetic field described by the following Hamiltonian

3.1 Spin chain in magnetic field

\[ H = H_0 + \alpha \sigma_z \rho. \]

Because of errors of quantum calculations we obtain imaginary part of\( \sigma_z \) which looks as a noise. Therefore on Fig. 3 we present the real part of\( \sigma_z \). Also, with exactness to total phase factor we use representation of\( \exp(-i \tau \sigma_z^t \hbar) \) as a target. Also, with exactness to total phase factor we use representation of\( \exp(-i \tau \sigma_z^t \hbar) \) asCNOT\( \alpha \) and perform calculations for\( \alpha/2 = Jt/\hbar \) changing from\(-8\pi/24\) to\( 8\pi/24 \) with the step\( \pi/24 \).

The quantum protocol for the studies is given on Fig. 2. Constructing the quantum protocol we take into account that with exactness to total phase factor operator\( \exp(-i J \sigma_z^t \hbar) \) can be represented as CNOT\( jk \) RZ\( k \) (2\( Jt/\hbar \)) CNOT\( jk \), here RZ\( k \) (2\( Jt/\hbar \)) is the Z-rotation gate acting on qubit\( q[k] \), CNOT\( jk \) is the controlled-NOT gate (operator CNOT\( jk \) acts on\( q[j] \) as control and on\( q[k] \) as a target). Also, with exactness to total phase factor we use representation of\( \exp(-i J \sigma_z^t \hbar) \) asCNOT\( jk \) CNOT\( kl \) RZ\( k \) (2\( Jt/\hbar \)) CNOT\( kl \) CNOT\( jk \) and take into account that (CNOT\( jk \))^2 = 1.

The results of detecting of the energy levels of the spin chain in the magnetic field are presented on Fig. 3. The value\( \sigma_z^t(\omega) \) is real. Because of errors of quantum calculations we obtain imaginary part of\( \sigma_z^t(\omega) \) which looks as a noise. Therefore on Fig. 3 we present the real part of\( \sigma_z^t(\omega) \) detected on the quantum device. The sharp peaks of\( \text{Re} \sigma_z^t(\omega) \) at points\( \omega = \pm 6, \omega = \pm 10, \omega = \pm 14, \omega = \pm 22 \) correspond to the energies\( E_T = \pm 3J, E_T = \pm 5J, E_T = \pm 7J, E_T = \pm 11J \) of the total Hamiltonian\( H_T (10) \).

Small peak at\( \omega = 0 \) appears in\( \text{Re} \sigma_z^t(\omega) \) obtained on the basis of quantum calculations on ibmq-bogota Fig. 3c and is absent on Fig. 3b corresponding to results obtained on the quantum simulator. This peak is related with systematic error shift of the results of quantum calculations for\( \sigma_z^t(\omega) \). Energy spectrum of the total Hamiltonian (10) contains positive eigenvalues of\( H + C \) and eigenvalues of\( -(H + C) \) which are negative and does not contain\( E_T = 0 \). So, the peak at\( \omega = 0 \) has not to be taken into account. Using relation of\( H_T (10) \) with the Hamiltonian of the system\( H(9) \) we find the following results for the energy levels of the spin chain in the magnetic field\( E = -3J, E = -J, E = J, E = 5J \). The obtained spectrum corresponds to the analytical one.

At the end of this subsection we would like to note that in (9) the coupling strength was chosen to be equal to the magnetic field for convenience. The method can be applied for arbitrary value of the coupling strength.

3.2 Triangle spin cluster

As the next example we consider triangle spin cluster described by the following Hamiltonian

\[ H = J \sigma_1^x \sigma_2^x + J \sigma_2^x \sigma_3^x + J \sigma_3^x \sigma_1^x + J \sigma_1^z + J \sigma_2^z + J \sigma_3^z. \]

It is worth mentioning that to detect all peaks representing the eigenvalues of\( H_T \) in the Fourier transformation the time interval\( \tau \) has to be chosen to satisfy the following inequality\( \tau = \pi/2\omega_{\text{max}}^T \). Here\( \omega_{\text{max}}^T \) is the maximal eigenvalue of\( H_T \) in units of\( \hbar \),\( E_{\text{max}}^T = \hbar \omega_{\text{max}}^T \) [25]. The delta-peaks are more thin and more higher for larger\( N \tau \).

In the next section we detect the energy levels of spin systems on IBM’s quantum computer on the basis of studies of evolution of mean value of probe spin using quantum protocol Fig. 1.

3 Estimation of the energy levels of spin systems by studies of a probe spin evolution on IBM's quantum computer

3.1 Spin chain in magnetic field

Let us consider a spin chain in magnetic field described by the following Hamiltonian

\[ H = J \sigma_1^x \sigma_2^x + J \sigma_2^y \sigma_3^y + J \sigma_1^z + J \sigma_2^z + J \sigma_3^z. \]

In this case the total Hamiltonian (2) reads

\[ H_T = J \sigma_0^z \sigma_1^z + \sigma_2^z \sigma_3^z + \sigma_1^z + \sigma_2^z + \sigma_3^z + C. \]

To provide the positivity of the energy levels of\( H \) the constant\( C \) is chosen to be\( C = 6 \). The initial state is considered as\( |++++\rangle \). We detect the mean value of\( \sigma_0^z \) on IBM’s quantum computer ibmq-bogota. For convenience we put\( J/\hbar = 1 \) and perform calculations for\( \alpha/2 = Jt/\hbar \) changing from\(-8\pi/24 \) to\( 8\pi/24 \) with the step\( \pi/24 \).

The quantum protocol for the studies is given on Fig. 2. Constructing the quantum protocol we take into account that with exactness to total phase factor operator\( \exp(-i J \sigma_z^t \hbar) \) can be represented as CNOT\( jk \) RZ\( k \) (2\( Jt/\hbar \)) CNOT\( jk \), here RZ\( k \) (2\( Jt/\hbar \)) is the Z-rotation gate acting on qubit\( q[k] \), CNOT\( jk \) is the controlled-NOT gate (operator CNOT\( jk \) acts on\( q[j] \) as control and on\( q[k] \) as a target). Also, with exactness to total phase factor we use representation of\( \exp(-i J \sigma_z^t \hbar) \) asCNOT\( jk \) CNOT\( kl \) RZ\( k \) (2\( Jt/\hbar \)) CNOT\( kl \) CNOT\( jk \) and take into account that (CNOT\( jk \))^2 = 1.

The results of detecting of the energy levels of the spin chain in the magnetic field are presented on Fig. 3. The value\( \sigma_z^t(\omega) \) is real. Because of errors of quantum calculations we obtain imaginary part of\( \sigma_z^t(\omega) \) which looks as a noise. Therefore on Fig. 3 we present the real part of\( \sigma_z^t(\omega) \) detected on the quantum device. The sharp peaks of\( \text{Re} \sigma_z^t(\omega) \) at points\( \omega = \pm 6, \omega = \pm 10, \omega = \pm 14, \omega = \pm 22 \) correspond to the energies\( E_T = \pm 3J, E_T = \pm 5J, E_T = \pm 7J, E_T = \pm 11J \) of the total Hamiltonian\( H_T (10) \).

Small peak at\( \omega = 0 \) appears in\( \text{Re} \sigma_z^t(\omega) \) obtained on the basis of quantum calculations on ibmq-bogota Fig. 3c and is absent on Fig. 3b corresponding to results obtained on the quantum simulator. This peak is related with systematic error shift of the results of quantum calculations for\( \sigma_z^t(\omega) \). Energy spectrum of the total Hamiltonian (10) contains positive eigenvalues of\( H + C \) and eigenvalues of\( -(H + C) \) which are negative and does not contain\( E_T = 0 \). So, the peak at\( \omega = 0 \) has not to be taken into account.

Using relation of\( H_T (10) \) with the Hamiltonian of the system\( H(9) \) we find the following results for the energy levels of the spin chain in the magnetic field\( E = -3J, E = -J, E = J, E = 5J \). The obtained spectrum corresponds to the analytical one.

At the end of this subsection we would like to note that in (9) the coupling strength was chosen to be equal to the magnetic field for convenience. The method can be applied for arbitrary value of the coupling strength.
Results of quantifying of the energy levels of spin chain in the magnetic field (9). Evolution of the mean value $\langle \sigma^x_0 \rangle$ detected on ibmq-bogota (a). The real part of $\sigma^x_0(\omega)$ obtained on the basis of the results of calculation of $\sigma^x_0(t)$ on ibmq-qasm-simulator (b) and on ibmq-bogota (c). The peaks of $\text{Re} \sigma^x_0(\omega)$ at $\omega = \pm 6, \omega = \pm 10, \omega = \pm 14, \omega = \pm 22$ correspond to energies $E_T = \pm 3J, E_T = \pm 5J, E = \pm 7J, E = \pm 11J$ of the total Hamiltonian (10) and energies $E = -3J, E = -J, E = J, E = 5J$ of the spin chain in the magnetic field (9). The dimensionless time $t$ is defined in units $\hbar/J$ and the dimensionless frequency $\omega$ is defined in units $J/\hbar$.

Choosing $C = 7$, we can write the expression for the total Hamiltonian as

$$H_T = J\sigma^z_0(\sigma^z_1\sigma^z_2 + \sigma^z_2\sigma^z_3 + \sigma^z_3\sigma^z_1 + \sigma^z_1 + \sigma^z_2 + \sigma^z_3 + 7).$$

Quantum protocol for studies of the mean value of $\sigma^x_0$ in the case of the triangle spin cluster is presented on Fig. 4.

The results of quantum calculation of the mean value of $\sigma^x_0$ for $\alpha/2 = Jt/\hbar$ changing from $-8\pi$ to $8\pi$ with the step $\pi/30$ are presented on Fig. 5a. On Fig. 5 we present $\text{Re} \sigma^x_0(\omega)$ obtained on the basis of calculation on ibmq-qasm-simulator (b) and on ibmq-bogota (c).
Fig. 5 Results of quantifying of the energy levels of triangle spin cluster (11). Evolution of the mean value $\langle \sigma^x_0 \rangle$ detected on ibmq-bogota (a). The real part of $\sigma^x_0(\omega)$ obtained on the basis of calculations of $\sigma^x_0(t)$ on ibmq-qasm-simulator (b) and on ibmq-bogota (c). The peaks of $\text{Re}\sigma^x_0(\omega)$ at $\omega = \pm 10, \omega = \pm 14, \omega = \pm 26$ correspond to energies $E_T = \pm 5J, E_T = \pm 7J, E_T = \pm 13J$ of the total Hamiltonian (12) and energies $E = -2J, E = 0, E = 6J$ of the triangle spin cluster (11). The dimensionless time $t$ is defined in units $\hbar/J$ and the dimensionless frequency $\omega$ is defined in units $J/\hbar$.

In addition we consider triangle spin cluster with spatial anisotropic interaction described by the Hamiltonian

$$H = -J\sigma^x_1\sigma^x_2 + J\sigma^x_2\sigma^x_3 + J\sigma^x_1\sigma^x_3 + J\sigma^z_1 + J\sigma^z_2 + J\sigma^z_3.$$  \hfill (13)

Similarly as in the previous case, choosing $C = 7$ the expression for the total Hamiltonian reads

$$H_T = J\sigma^x_0(-\sigma^z_1\sigma^z_2 + \sigma^z_2\sigma^z_3 + \sigma^z_1\sigma^z_3 + \sigma^z_1 + \sigma^z_2 + \sigma^z_3 + 7).$$  \hfill (14)

ibmq-bogota (c). The sharp peaks of $\text{Re}\sigma^x_0(\omega)$ at the points $\omega = \pm 10, \omega = \pm 14, \omega = \pm 26$, correspond to the total Hamiltonian $H_T$ energies $E_T = \pm 5J, E_T = \pm 7J, E_T = \pm 13J$, respectively. Therefore for the triangle spin cluster we obtain energy levels as follows $E = -2J, E = 0, E = 6J$. The result is in agreement with the theoretical one. Similarly as in the previous example, the peak at $\omega = 0$ Fig. 5c is related with quantum errors and has not to be taken into account.
Fig. 6 Results of quantifying of the energy levels of triangle spin cluster with spatial anisotropic interaction (13). Evolution of the mean value $\langle \sigma_x^0 \rangle_{\text{detected}}$ on ibmq-bogota (a). The real part of $\sigma_x^0 (\omega)$ obtained on the basis of calculations of $\sigma_x^0 (t)$ on ibmq-qasm-simulator (b) and on ibmq-bogota (c). The peaks of $\text{Re} \, \sigma_x^0 (\omega)$ at $\omega = \pm 6, \omega = \pm 10, \omega = \pm 14, \omega = \pm 18, \omega = \pm 22$ correspond to energies $E_T = \pm 3J, E_T = \pm 5J, E_T = \pm 7J, E_T = \pm 11J$ of the total Hamiltonian (14) and energies $E = -4J, E = -2J, E = 0, E = 4J$ of the triangle spin cluster with spatial anisotropic interaction (13). The dimensionless time $t$ is defined in units $\bar{h}/J$ and the dimensionless frequency $\omega$ is defined in units $J/\bar{h}$.

The evolution of the mean value of $\sigma_0^X$ was studied for $\alpha/2 = Jt/\bar{h}$ changing from $-\pi$ to $\pi$ with the step $\pi/30$ using quantum protocol Fig. 4 with changing the sign of the parameter $\alpha$ in the first $RY$ gate acting on $q[2]$ to the opposite one. The obtained results are presented on Fig. 6. On Fig. 6b, c we see peaks of $\text{Re} \sigma_x^0 (\omega)$ at $\omega = \pm 6, \omega = \pm 10, \omega = \pm 14, \omega = \pm 18, \omega = \pm 22$. They correspond to energies $E_T = \pm 3J, E_T = \pm 5J, E_T = \pm 7J, E_T = \pm 11J$ of the total Hamiltonian (14), respectively. So, on the basis of the quantum calculations we obtain the energy levels of the triangle spin cluster with spatial anisotropic interaction (13) as follows $E = -4J, E = -2J, E = 0, E = 4J$ as it should be according to the analytical calculations. The peak at $\omega = 0$ Fig. 6c is related with quantum errors and has not to be considered.
3.3 Ising model on squared lattice in the magnetic field

In this subsection we present results of detection of the energy levels of the Ising model on squared lattice in the magnetic field (15) are presented on Fig. 8. Similarly as in the previous examples for convenience we put \( J = \sqrt{2}, \) \( \bar{h} = 2, \) \( C = 9, \) \( \alpha = 2Jt/h \) changing from \( -8\pi \) to \( 8\pi \) with the step \( \pi/36. \) The results of detection of the energy levels of the Ising model on squared lattice in the magnetic field (15) are presented on Fig. 8. Similarly as in the previous examples for convenience we put \( J/h = 1. \) The peaks of \( \text{Re} \sigma_3^0(\omega) \) at \( \omega = \pm 10, \) \( \omega = \pm 14, \) \( \omega = \pm 18, \) \( \omega = \pm 22, \) \( \omega = \pm 34 \) correspond to the total Hamiltonian \( H_T \) energies \( E_T = \pm 5J, \) \( E_T = \pm 7J, \) \( E_T = \pm 9J, \) \( E_T = \pm 11J, \) \( E_T = \pm 17J. \) Similarly as in the previous cases the peak at \( \omega = 0 \) Fig. 8c is related with quantum errors and has not to be taken into account. So, the detected energy levels of Ising square lattice in the magnetic field read \( E = -4J, \) \( E = -2J, \) \( E = 2J, \) \( E = 8J. \) The obtained results for the energy levels correspond the the analytical ones.

3.4 A spin in magnetic field

Let us study energy levels of a spin in a magnetic with the following Hamiltonian \( H = J(\mathbf{n} \cdot \mathbf{\sigma}) \). We consider \( \mathbf{n} = (1/\sqrt{2}, 1/\sqrt{2}, 0), \)

\[
H = J \sqrt{2} (\sigma_1^x + \sigma_1^z).
\]

(17)

Note that the terms in (17) do not commute. The total Hamiltonian reads

\[
H_T = J/\sqrt{2} (\sigma_0^x \sigma_1^x + \sigma_0^z \sigma_1^z) + CJ\sigma_0^z
\]

(18)

Quantum protocol for studies of evolution of \( \sigma_0^z \) operator is presented in Fig. 9

In (9) we consider the initial state to be

\[
|\psi_0\rangle = \frac{1}{2} (|0\rangle_0 + |1\rangle_0) \left( |0\rangle_1 + e^{i\pi/2} |1\rangle_1 \right) = H_0 H_1 P \left( \frac{\pi}{4} \right) |00\rangle.
\]

(19)

We also take into account that the operator of evolution \( \exp(-iHt/h) \) can be represented as

\[
\exp \left( -\frac{iHt}{h} \right) = U \left( -\frac{2Jt}{h}, \frac{3\pi}{4}, \frac{3\pi}{4} \right).
\]

(20)

where \( U(\theta, \phi, \lambda) \) is the U-gate

\[
U(\theta, \phi, \lambda) = RZ(\phi - \pi/2) RX(\pi/2) RZ(\pi - \theta) RX(\pi/2) RZ(\lambda - \pi/2).
\]

(21)

Creating protocol Fig. 9, we also use the following representation

\[
\exp(-iH_t/h) = U_1 \left( -\theta, \frac{3\pi}{4}, \frac{3\pi}{4} \right) \left( 2\theta, \frac{3\pi}{4}, -\frac{3\pi}{4} \right) RZ(C\theta),
\]

(22)

where \( U_1(-\theta, 3\pi/4, -3\pi/4) \) is the U-gate (21) acting on the state of qubit \( q[1], \) \( \text{CU}_{01}(2\theta, 3\pi/4, -3\pi/4) \) is the controlled U-gate that acts on qubit \( q[0] \) as control and on qubit \( q[1] \) as target, \( \theta = 2Jt/h. \)

Quantum protocol Fig. 9 was realized on ibmq-bogota changing \( \theta/2 = Jt/h \) from \( -8\pi \) to \( 8\pi \) with the step \( \pi/24 \) and choosing constant \( C = 2 \) (in this case the energy levels of \( H \) are positive). The results of calculation of the mean value of \( \sigma_0^z \) on IBM’s quantum computer are presented in Fig. 10. We put \( J/h = 1. \) Clear peaks at \( \omega = \pm 2, \omega = \pm 6, \) correspond to the energies of the total Hamiltonian \( E_T = \pm J, \) \( E_T = \pm 3J \) and energies \( E = -J, E = J \) of the spin in the magnetic field (17).
Fig. 8 Results of quantifying of the energy levels of Ising model on squared lattice in the magnetic field (15). Evolution of the mean value $\langle \sigma_x^0 \rangle$ detected on ibmq-bogota (a). The real part of $\sigma_x^0(\omega)$ obtained on the basis of the results of calculations of $\sigma_x^0(t)$ on ibmq-qasm-simulator (b) and on ibmq-bogota (c). The peaks of $\text{Re} \sigma_x^0(\omega)$ at $\omega = \pm 10$, $\omega = \pm 14$, $\omega = \pm 18$, $\omega = \pm 22$, $\omega = \pm 34$ correspond to energies $E_T = \pm 5J$, $E_T = \pm 7J$, $E_T = \pm 9J$, $E_T = \pm 11J$, $E_T = \pm 17J$ of the total Hamiltonian (16) and energies $E = -4J$, $E = -2J$, $E = 0$, $E = 2J$, $E = 8J$ of the Ising model on squared lattice in the magnetic field (15). The dimensionless time $t$ is defined in units $\hbar/J$ and the dimensionless frequency $\omega$ is defined in units $J/\hbar$.

Fig. 9 Quantum protocol for studies of evolution of mean value of $\sigma_x^0$ in the case of spin in the magnetic field (17) on a quantum computer. Here $C = 2$, $\theta = 2Jt/\hbar$, $\psi = 3\pi/4$. 

$q[0] |0\rangle$ 
\[ H \]
$q[1] |0\rangle$ 
\[ H \]
$P_\pi$ 
\[ U_{\theta,\pi,0} \]
\[ U_{2\theta,\pi,0} \]
\[ R_{Z}(2\pi) \]
\[ R_{Y}(\pi) \]
Fig. 10 Results of quantifying of the energy levels of the spin in the magnetic field (17). Evolution of the mean value $\langle \sigma_x^0 \rangle$ detected on ibmq-bogota (a). The real part of $\sigma_x^0 (\omega)$ obtained on the basis of the results of calculations of $\sigma_x^0 (t)$ and on ibmq-bogota (b). The peaks of $\text{Re} \, \sigma_x^0 (\omega)$ at $\omega = \pm 2$, $\omega = \pm 6$ correspond to energies $E_T = \pm J$, $E_T = \pm 3J$ of the total Hamiltonian (18) and energies $E = -J$, $E = J$ of the spin in the magnetic field (17). The dimensionless time $t$ is defined in units $\hbar / J$ and the dimensionless frequency $\omega$ is defined in units $J / \hbar$.

At the end of this section we would like to note that in the case of a spin in the magnetic field we have represented the operator of evolution with the unitary gate (20). In general case for realization of the operator of evolution the Trotterization procedure can be used. Namely, if the Hamiltonian of a system contains terms $H_k$ that do not commute $H = \sum_k H_k$ the operator of evolution can be written as

$$\exp \left( -it \sum_k H_k / \hbar \right) = \lim_{n \to \infty} \left( \prod_k \exp \left( -it H_k / n \hbar \right) \right)^n. \tag{23}$$

So, the operator of evolution with Hamiltonian $H$ can be represented as the product of operators of evolution with terms $H_k$ that can be realized on a quantum devise. On a quantum computer we can realize a finite number of operators (finite $n$). It is important to note that the representation of the operator of evolution is more accurate for large $n$, at the same time in this case the number of gates for realization of the operator of evolution is also large that leads to accumulating of gate errors. Therefore for particular problem and particular device the optimal $n$ can be found. We hope that with developing of multi-qubit quantum computers with large quantum volumes the operator of evolution can be realized with height accuracy on the basis of the Trotterization procedure.

4 Conclusions

The method of detecting of the energy levels of a spin system on the basis of studies of evolution of a probe spin has been proposed. The method provides possibility to estimate energy levels of many-spin system studying evolution of the mean value of only one probe spin and can be applied for arbitrary spin systems.

We have realized the proposed algorithm on IBM’s quantum computer ibmq-bogota and have detected the energy levels of spin systems with Ising interaction (a spin chain in the magnetic field, triangle spin cluster, Ising model on squared lattice in the magnetic field, a spin in the magnetic field). The results of quantum calculations (see Figs. 3, 5, 6, 8, 10) are in agreement with the theoretical ones. We would like to note that the method can be used for arbitrary Hamiltonian with commuting and anticommuting terms. Depending on the Hamiltonian the evolution operator can be realized on a quantum computer with a unitary gate (see example of a spin in the magnetic field (17)). In general the operator of evolution can be realized with a Trotterization procedure.
On the basis of the obtained results we conclude that the method is efficient even in the case of noisy quantum devices. The advantage of the proposed method is that for detection of the energy levels we use only one ancilla qubit and do not need to measure the states of all qubits. The quantum protocol Fig. 1 contains only measurement of one qubit which leads to reduction of the readout errors. The proposed method is efficient for estimation of the energy levels of many spin systems. Besides it is worth stressing that it is nontrivial combinatorial optimization problem to find minimal or maximal eigenvalue of the Ising model in the case when the constants $J_{ij}$ in (4) are different. Therefore the proposed method opens a possibility to achieve quantum supremacy in solving eigenvalue problem with development of multi-qubit quantum computers.

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