of a quantum computer?'' has never yet been addressed in the literature but will become important one day for those who plan to set up the first experiment.

It is very likely that the first experimental proof-of-principle study will start with simple one-qubit operations. Therefore, in this paper we focus on a one vibrational degree of freedom example i.e., a one-qubit system). Instead of attacking any particular molecule or any particular normal mode in a chosen real world molecule, we consider a model system where we are free to vary, in

ample, for the gate NOT we have to find a pulse, which induces not just one, but two transitions

where , is harmonic frequency and[is the anharmonicity parameter defined as

$$, \quad a\sqrt{\frac{2D}{m}}, \quad [\quad \frac{a^2}{2m}. \qquad 11)$$

All of the necessary Morse

Figures 3 a)–3 d) illustrate our results for this gate in the OH diatomic compare to Figs. 2 a)–2 d) for the gate NOT]. Although the general shape of the Hadamard pulse is very similar to the shape of the NOT pulse, the field amplitude is about twice smaller in the case of the Hadamard gate note different scales in Figs. 2 a) and 3 a)]. This

Kutta method.[21] We employed the interaction representation to analytically factor out all oscillatory phases; this way we are able to use a larger time step ($\Delta t = 10$ a.u.). The dipole-moment matrix elements $\mu_{ij} = \langle \psi_j(r) | \mu(r) | \psi_i(r) \rangle$ are computed only once and are stored in memory. Therefore, we suggest that basis set expansion is the method of choice for the numerical modeling of

section. As expected, the highest fidelity in each case is achieved with the highest value of[$=110\ \mathrm{cm}^{-1}$. It is $P_{i,f}^{1,2}$ $=0.994\,867$ for the gate NOT and $P_{i,f}^{1,2}=0.998\,762$ for the Hadamard transform. One important finding is the presence of a high fidelity plateau in the region 50 [110 cm^{-1}. The results for the real OH molecule, discussed in detail in the preceding section (90 cm^{-1}), are shown as filled symbols in the insert in Fig. 4 and fall onto that

states in the process, which in turn increases the fidelity of qubit transformation.

By analogy with Fig. 6 we

onstrated that a number of factors can and should be employed in order to achieve the high fidelity of gates in such a quantum computer. One of these factors is the anharmonicity parameter of the molecule itself. Indeed, we have observed the high fidelity plateau in the region 50 [110 cm^{-1}. In such anharmonic systems, it is easier to achieve a good control over the vibrational processes because the different state-to-state transitions are easier to resolve and, as we have shown, it is easier to restrict the vibrational population of the molecule to the qubit states $|0\rangle$ and $|1\rangle$. Therefore, we suggest that using molecules with large anharmonicity parameters will help significantly in achieving the necessary high fidelity of gates in the vibrational qubit. The anharmonicity parameter of the OH diatomic is[90 cm^{-1}, and falls into that range. Naturally, all bonds that involve hydrogen atom are very anharmonic and are good candidates for implementing a vibrational qubit. For example, the anharmonicity parameter of the CH diatomic is[63 cm^{-1} and is also in that range. Among larger real world molecules many hydrocarbons benzene, naphthalene, etc.) can be good candidates for practical realization of multiple vibrational qubits. In such molecules, there are always several bright IR-active normal vibrational modes associated with CH stretches and those are very anharmonic. Other good candidates can, probably, be found among the molecules that have very unharmonic triple C O bonds, such as $Rh(CO)_2(C_5H_7O_2)$ Ref. 23) or $Cr(CO)_6$.[24]

We have observed that the fidelity of quantum gates drops significantly when the anharmonicity parameter is less than[$=40$ cm^{-1}. However, we have also found that even in such cases the fidelity of gates can be improved significantly by relaxing constraints on the shaped pulse. Thus, longer pulses allow using a field of smaller amplitude and avoid putting too much population into the upper vibrational states $|2\rangle$, $|3\rangle$, $|4\rangle$,...) interfering with the states of the qubit $|0\rangle$ and $|1\rangle$. This permits to use efficiently the molecules with not enough anharmonicity and obtain a much better fidelity of quantum gates.

The effect of the penalty function used to smoothly switch-on and switch-off the optimal pulse is somewhat similar to reducing the pulse duration and is, therefore, negative in a sense of the gate fidelity. Thus, the $\sin^2$ penalty function 3) rises and decays, perhaps too slowly, reaching the unit value only in the middle of the pulse ($t=T/2$) and leaving a very short time for efficient pulse action. This must be compensated by increasing the field amplitude, which increases the population of upper vibrational states and results in lower fidelity of the gates. Therefore, we suggest exploring other forms of the penalty function in order to meet both conditions simultaneously: the smoothly switching-on and switching-off of the pulse and the relatively long time of efficient pulse action. This can be easily achieved with penalty functions that are flatter than the $\sin^2$ function in Eq. 3).

Furthermore, we have clearly seen that some quantum gates exhibit naturally better fidelity than the others. In all cases considered here the fidelity of the Hadamard rotation was significantly better than the fidelity of the gate NOT. This is because for the Hadamard rotation we need to transfer only $\frac{1}{2}$ of the population between the qubit states. This is achieved using the field of smaller amplitude and results in better gate fidelity.

Finally, we have demonstrated that a quantum computer based on vibrational eigenstates to implement the quantum information bits and optimally shaped laser pulses to apply the quantum logic gates can be a robust tunable system. Carefully choosing various properties of the molecule and of the pulse allows one to achieve very high fidelity gates.

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