Atomic wave packet basis for quantum information

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We propose a wave packet basis for storing and processing several qubits of quantum information in a single multilevel atom. Using radially localized wave packet states in the Rydberg atom, we construct an orthogonal basis that is related to the usual energy level basis by a quantum Fourier transform. A transform-limited laser pulse that is short compared with the classical Kepler period of the system interacts mainly with the wave packet state localized near the atomic core, allowing selective control in this basis. We argue that wave packet control in this regime is useful for multilevel quantum information processing.

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Quantum information processing is a growing interdisciplinary field that has seen rapid progress in the last few years [1]. However physical implementations of large scale quantum networks are severely limited by decoherence [2], the loss of coherence in the superposition state of the system. This is especially true of extended systems that involve entanglement of macroscopic degrees of freedom, such as the center-of-mass motion of atoms in a trap [3].

We consider multiple computational levels in each atom to store information more densely. The radiative lifetime of Rydberg levels scales as n^3, where n is the principal quantum number, and approaches a millisecond for $n > 100$. In most atomic quantum logic schemes, the bottleneck for the coherence time is the macroscopic entanglement of two or more atoms. The multilevel approach minimizes this decoherence by reducing the number of atoms in the quantum network, with each d-level atom representing $\log_2 d$ qubits of information [4]. In a $d = 8$ level scheme, for example, the number of atoms that need to be entangled is less by a factor of three.

A great deal of research has been carried out in the past few years developing techniques for controlling multilevel Rydberg wave packets using shaped short pulses. It is attractive to exploit this work by developing an alternative wave packet basis for the quantum information stored in the atomic energy levels. Rydberg wave packets are coherent superpositions of atomic energy eigenstates with large principal quantum numbers. We can use the relative phases of the different eigenstates in the superposition to store information. Using the energy-time Fourier kernel in unitary time evolution, we define an orthogonal, discrete wave packet basis that is related to the energy levels by a quantum Fourier transform. This transform plays a key role in quantum computing applications [5], and we show how it naturally permits complementary bases for representing the information stored in a multilevel quantum system.

In the optical domain, a discrete Fourier transform connects the spectral and temporal modes of the radiation field in a cavity. Iaconis et al. [6] use this approach to characterize the Husimi distribution of a multimode quantum field in heterodyne detection. Tittel et al. [7] exploit the complementarity of energy and time in their scheme for quantum cryptography using entangled photons. In the atomic case, Muller and Noordam [8] introduce a Fourier relation between the energy quantum number and a continuous phase coordinate to study the photoexcitation of Rydberg states. We show how the quantum Fourier transform of the energy levels corresponds exactly to a discrete temporal basis of wave packets in cyclic motion about the nucleus.

We consider radial wave packets, which are superpositions of Rydberg states with low angular momentum. These states are radially localized in probability and evolve periodically for short times, or in the classical correspondence limit [9]. The wave packet basis we introduce corresponds to discrete times in this classical evolution, when each wave packet state is centered at a different radius from the atomic nucleus. This basis is non-stationary in time, with wave function amplitudes evolving cyclically during a classical period. Due to the unequal spacing of the energy levels, the wave function undergoes dispersion, which leads to revivals and super revivals in the wave packet amplitudes. The classical motion and quantum revival structure of this free time evolution allows for the possibility of conveniently controlling the wave function at suitably chosen intervals of time.

We propose using short optical pulses to couple coherently the Rydberg manifold to a low-lying energy level in the atom. A transform-limited pulse that is short compared to the classical Kepler period of the system interacts with all the energy levels but couples only to the wave packet state that is nearest the atomic core, a phenomenon familiar in the excitation and photoionization of Rydberg states [10]. The classical electron has the largest momentum, and hence absorbs energy most efficiently, when near the core. During the pulse, the wave packet state nearest the nucleus and the ground state form an effectively two-level system, and undergo Rabi oscillations.

Coherent control of wave packets based on spatial localization has been studied by Ahn et al. [11], who show that half-cycle pulses can be used to extract binary phase information stored in a radial wave packet. The use of optical pulses shorter than a Kepler period for quantum control of atomic wave packets in the strong-field regime has been studied analytically by Araujo et al. [12]. A weak field analysis by Noel and Stroud [13] showed that a uniform train of d pulses within one Kepler period can be used to create an arbitrary Rydberg state of d levels whose amplitudes are related by a discrete Fourier transform to the pulse amplitudes. We propose to use such pulses for selective processing of quantum information in the wave packet basis.

Consider d Rydberg energy levels with angular momentum $l = 1$ in a hydrogen or alkali atom as a quantum information basis,

$$|j\rangle_\nu = |\bar{n} + j, 1, 0\rangle, \qquad (1)$$
$$j = -d/2 + 1, -d/2 + 2, \ldots, d/2,$$

where $\bar{n}$ is the mean value for the principal quantum number in the wave packet superposition, and the subscript ν is used to denote a state in the energy basis. We have assumed above that the number of levels d is an even number, but the arguments below are easily extended to odd d. These levels can be excited simultaneously from the ground state by a strong linearly polarized laser pulse with sufficient bandwidth to overlap all the levels. The pulsed excitation creates a wave packet which evolves in time as

$$|\psi(t)\rangle = \sum_n b_j \exp(-i\omega_j t)\,|j\rangle_\nu, \qquad (2)$$

where $\hbar\omega_j$ is the energy of the jth Rydberg level and the amplitudes b_j are determined by the spectrum of the exciting pulse. If we assume that the pulse spectrum, centered at ω_0, is uniform over the d computational levels and falls off rapidly outside this manifold, we have a uniform amplitude distribution, $b_j = 1/\sqrt{d}$, which is time independent in the absence of external fields.

The radial wave packet was first studied by Parker and Stroud [9], who showed that it corresponds to a radially localized shell of probability distribution moving periodically between the classical turning points for short times. Eventually, the uneven spacing in the energies of the levels in Eq. (1) leads to dispersions and revivals of the wave packet, corresponding to the time-dependent phases in Eq. (2) interfering destructively or constructively. The rates at which the phases evolve with respect to each other depend on the frequencies ω_j relative to the average frequency ω_0, which can be expanded in a Taylor series in $j = n - \bar{n}$,

$$\omega_{j0} = \omega_j - \omega_0 = -\frac{1}{2(\bar{n}+j)^2} + \frac{1}{2\bar{n}^2}$$
$$= 2\pi\left[\frac{j}{T_K} - \frac{j^2}{T_{\rm rev}} + \frac{j^3}{T_{\rm sr}} - \cdots\right], \qquad (3)$$

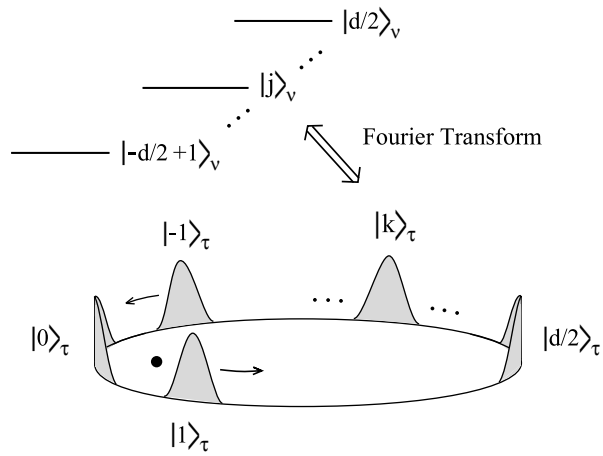

FIG. 1. Illustration of conjugate bases: Energy eigenstates $|j\rangle_\nu$ related by a Fourier transform to wave packet states $|k\rangle_\tau$ evenly distributed in time around a classical orbit. A radial wave packet basis can be thought of as an ensemble of such orbits with different orientations for the ellipses.

where in atomic units, $T_K = 2\pi\bar{n}^3$ is the classical Kepler period for round trip motion, $T_{\rm rev}/2! = 2\pi\bar{n}^4/3$ is when the wave packet revives first, $T_{\rm sr}/3! = \pi\bar{n}^5/6$ is when the wave packet super-revives first, etc. At $\bar{n} = 180$ for example, $T_K \simeq 0.89$ ns, $T_{\rm rev} \simeq 106$ ns, and $T_{\rm sr} \simeq 14$ μs. For large $\bar{n}$, the different time scales are well separated in magnitude, and for a small number of levels d, the wave packet is more spread out in space and disperses more slowly in time. For $d^2 \ll \bar{n}$, we see from Eq. (3) that the revival dynamics of the wave packet can be neglected to good approximation during the first few Kepler periods, and Eq. (2) becomes

$$|\psi(t)\rangle \approx \frac{1}{\sqrt{d}}\sum_j \exp\left(-i2\pi jt/T_K\right)|j\rangle_\nu,$$
$$= |\psi_K(t)\rangle \qquad (4)$$

which evolves periodically in time with period T_K.

The Fourier kernel in Eq. (4) involves j and t, and can be thought of as underlying an uncertainty relation between energy and time, with more levels leading to greater spatio-temporal localization of the wave packet. Although the Rydberg energies are discrete, the time t for the wave packet varies continuously around the orbit. However, if we consider d discrete times during any Kepler period,

$$t_k = k(T_K/d), \qquad (5)$$
$$k = -d/2 + 1, -d/2 + 2, \ldots, d/2,$$

we can construct an alternate discrete wave packet basis $|k\rangle_\tau$ for the system of energy levels in Eq. (1) based on the quantum Fourier transform (QFT),

$$|k\rangle_\tau = |\psi_K(t_k)\rangle = \frac{1}{\sqrt{d}}\sum_j \exp\left(-i2\pi jk/d\right)|j\rangle_\nu. \quad (6)$$

This is an orthogonal basis in time (denoted by the subscript τ), and the basis amplitudes evolve periodically with the classical period T_K, as illustrated in Fig. 1. Thus $k = 0$ and $k = d/2$ correspond to wave packet states centered at the inner and outer turning points of the classical orbit respectively. The sign of k indicates the direction of propagation of the wave packet. We can also define the basis for odd d, except that in this case $k = \pm(d-1)/2$ correspond to wave packet states centered near (but not exactly at) the outer turning point, having nonzero and opposite momenta. The energy eigenstates can be recovered from $|k\rangle_\tau$ by an inverse QFT,

$$|j\rangle_\nu = \frac{1}{\sqrt{d}}\sum_k \exp\left(i2\pi jk/d\right)|k\rangle_\tau. \quad (7)$$

In general, any excited state $|\Psi(t)\rangle$ of the d Rydberg levels can be expanded in either basis,

$$|\Psi(t)\rangle = \sum_j b_j(t)\exp(-i\omega_j t)|j\rangle_\nu \quad (8)$$

$$= \exp(-i\omega_0 t)\sum_k \tilde{b}_k(t)|k\rangle_\tau, \quad (9)$$

where we have removed the center frequency ω_0 from the wave packet amplitudes $\tilde{b}_k$. A classical discrete Fourier transform (DFT) relates the two sets of amplitudes,

$$\tilde{b}_k(t) = \frac{1}{\sqrt{d}}\sum_j b_j(t)\exp(-i\omega_{j0}t)\exp\left(i2\pi jk/d\right). \quad (10)$$

For free time evolution, $b_j(t) = b_j(0)$, and Eq. (10) can be written as

$$\tilde{b}_k(t) = \sum_{k'} \tilde{b}_{k'}(0)\, u_{k'-k}(t), \quad (11)$$

where $u_{k'-k}(t)$ is the DFT of the time evolution kernel,

$$u_{k'-k}(t) = \frac{1}{d}\sum_j \exp\left[-i\omega_{j0}t - i2\pi j(k'-k)/d\right]. \quad (12)$$

In the Kepler regime of Eq. (3), the levels are equally spaced, $\omega_{j0} \simeq 2\pi j/T_K$, and $u_{k'-k}$ becomes a delta function in k', resulting in a cyclic permutation of the wave packet amplitudes in Eq. (11),

$$\tilde{b}_k(nT_K/d) = \tilde{b}_{k-n}(0), \quad (13)$$

where n is an integer and $k-n$ is taken modulo d. Equation (13) amounts to a SHIFT gate in the wave packet basis, the multivalued equivalent of the NOT gate for binary logic. More complex unitary transforms occur for longer times, when the revival and superrevival dynamics become relevant. Thus free time evolution alone becomes useful for quantum information processing in the wave packet basis. This is a consequence of the nonstationary character of the basis and the unequally spaced energy levels.

We now turn to the control of the multilevel atomic basis using laser fields. Universal multilevel transforms of the amplitudes b_j can in principle be achieved using narrow-band lasers to couple neighboring transitions among the energy levels [4]. However this requires multiple laser frequencies tuned to the $d-1$ transitions. A simpler control scheme is possible for the wave packet amplitudes $\tilde{b}_k$, as shown below. This involves short broadband pulses and takes advantage of the cyclic evolution of the wave packet states described above.

A laser pulse with a spectrum overlapping the d Rydberg levels couples most strongly to only that combination of the levels with a phase relation between them that localizes the electron near the core. This corresponds to the wave packet state $|0\rangle_\tau$, for which all the phases are equal since $k = 0$. Consider a pulsed field with a carrier frequency $\omega \approx \omega_0$ and pulse profile $f(t)$,

$$\mathbf{E}(t) = \boldsymbol{\epsilon} E_0 f(t)\exp(-i\omega t) + \text{c.c.}, \quad (14)$$

where E_0 and $\boldsymbol{\epsilon}$ are the amplitude and polarization of the field. Assume that the pulse couples the d Rydberg levels to the ground state $|g\rangle$ in the atom. In the energy level basis for the Rydberg states, the dipole interaction with the field yields the following coupled equations for time evolution in the rotating wave approximation,

$$\dot{b}_g = \frac{i}{2}f(t)\sum_j \Omega_j \exp(-i\Delta_j t)b_j, \quad (15)$$

$$\dot{b}_j = \frac{i}{2}f(t)\Omega_j \exp(i\Delta_j t)b_g, \quad (16)$$

where Ω_j and Δ_j are the Rabi frequency and field detuning defined as

$$\Omega_j = 2\langle g|\hat{\mathbf{d}}|j\rangle_\nu \cdot \boldsymbol{\epsilon} E_0/\hbar, \quad (17)$$

$$\Delta_j = \omega_j - \omega, \quad (18)$$

and we have taken Ω_j to be real in Eqs. (15) and (16). Using the Fourier inverse of Eq. (10), we rewrite the equation of motion for b_g in terms of the wave packet amplitudes,

$$\dot{b}_g = \frac{i}{2}f(t)\exp(-i\Delta_0 t)\sum_k \tilde{\Omega}_k \tilde{b}_k, \quad (19)$$

where Δ_0 is the mean detuning of the field, and $\tilde{\Omega}_k$ is the DFT of the Rabi frequency Ω_j,

$$\tilde{\Omega}_k = \frac{1}{\sqrt{d}}\sum_j \Omega_j \exp\left(-i2\pi jk/d\right). \quad (20)$$

To find the equation of motion for the wave packet amplitude $\tilde{b}_k$, we take the time derivative of Eq. (10) and

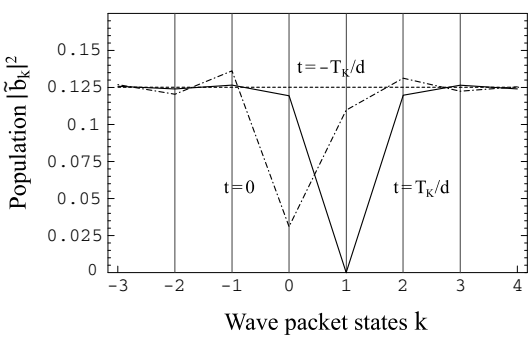

FIG. 2. Creation of a dark wave packet at $\bar{n} = 180$ and $d = 8$. The spectral width (FWHM) of the π pulse is approximately $1.3d/T_K$. The wave packet populations $|\tilde{b}_k|^2$ are shown before ($t = -T_K/d$), during ($t = 0$) and after ($t = T_K/d$) the pulse.

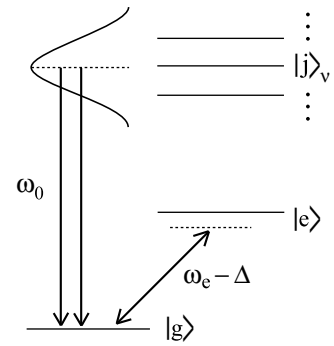

FIG. 3. Wave packet control for quantum information processing. The energy level basis is $|j\rangle_\nu = |\bar{n}+j, 1, 0\rangle$. Broadband π pulses de-excite two wave packet amplitudes in the conjugate wave packet basis. The ground levels g and e are coupled by a laser with frequency $\omega \approx \omega_e$.

use Eq. (16) for $\dot{b}_j$. Assuming that the pulse width is short compared to a Kepler period, we can ignore the free atomic evolution during the pulse that led to Eq. (11). In the short pulse regime, we are left with

$$\dot{\tilde{b}}_k = \frac{i}{2} f(t) \tilde{\Omega}_k^* \exp(i\Delta_0 t) b_g. \tag{21}$$

Equations (19) and (21) describe Rabi oscillations between the ground state and the wave packet states, where the Rabi frequencies $\tilde{\Omega}_k$ are Fourier transforms of their energy level counterparts Ω_j. For Rydberg levels, Ω_j varies slowly with j,

$$\Omega_j \sim (\bar{n}+j)^{-3/2}, \tag{22}$$

making only the dc component $\tilde{\Omega}_0$ significant for large $\bar{n}$. For $\bar{n} = 180$ and $d = 8$, we find $\tilde{\Omega}_{\pm 1} \simeq 0.01\ \tilde{\Omega}_0$. Thus to good approximation, we can ignore the Rabi frequencies $\tilde{\Omega}_{k\neq 0}$ in Eqs. (19) and (21). These equations reduce to

$$\dot{b}_g \cong \frac{i}{2} f(t) \tilde{\Omega}_0 \exp(-i\Delta_0 t) \tilde{b}_0, \tag{23}$$

$$\dot{\tilde{b}}_0 \cong \frac{i}{2} f(t) \tilde{\Omega}_0 \exp(i\Delta_0 t) b_g. \tag{24}$$

These describe two-level Rabi oscillations between the ground state and the innermost wave packet state during the pulse, with a detuning $\Delta_0 = \omega_0 - \omega$ between the peak of the pulse spectrum and the average Rydberg frequency. The two-level approximation is valid only for short pulses. To affect only the $k = 0$ wave packet state, we need the pulse width τ_p to be less than T_K/d, the time taken for this wave packet element to leave the atomic core. However, the bandwidth of the pulse cannot be much larger than the atomic frequencies spanning the d-level basis, to avoid coupling into levels outside this basis. Since the Rydberg frequency spacing is approximately $1/T_K$, this implies a bandwidth $\Delta\omega/2\pi \simeq d/T_K$. To summarize, we require that

$$\tau_p < \frac{T_K}{d} \simeq \frac{2\pi}{\Delta\omega}, \tag{25}$$

or that the pulse be transform-limited. For $\bar{n} = 180$ and $d = 8$ levels, we use a Gaussian pulse of width $\tau_p = 0.5 \ln 2\ T_K/d \simeq 110$ ps (FWHM amplitude), corresponding to a spectral width $\Delta\omega/2\pi = (8/2\pi)\ d/T_K$ for the electric field. Figure 2 shows an exact numerical solution for the wave packet amplitudes before, during and after the pulse. Assuming that the population is uniformly distributed initially, we find that a π pulse transfers nearly all the population in the $k = 0$ state to the ground state, creating a "dark" wave packet in the Rydberg basis that evolves cyclically in the Kepler evolution. About 5% of the population is lost from neighboring states $k = \pm 1$ during the pulse. Thus a coherent coupling of individual wave packet states with the ground state can be modeled as a two-level system to good approximation.

Since the wave packet basis is nonstationary in time, the Rydberg wave function undergoes dispersion and revivals as the energy level phases evolve in the Schrödinger picture. This leads to aperiodicity in the free time evolution of the wave packet amplitudes $\tilde{b}_k$, going beyond the cyclic regime of Eq. (13). At $\bar{n} = 180$ and $d = 8$ for example, we find that the population in a wave packet state decays by about 5% after a Kepler period, but recovers to within 2-4% at a revival or super-revival. This scales as $\bar{n}^{-2}$, making dispersion losses less significant for larger $\bar{n}$. By appropriate timing of successive laser pulses, we can thus take advantage of the revival structure of the atomic energy spectrum when addressing the wave packet amplitudes in the basis.

An arbitrary unitary transform of the d wave packet states can be decomposed into a product of $\mathcal{O}[d^2]$ two-dimensional transforms [14], each of which can be implemented sequentially on two de-excited wave packet amplitudes at a time, as shown in Fig. 3. Two low lying energy levels g and e temporarily store the wave packet amplitudes in the form $\tilde{b}_k|g\rangle + \tilde{b}_{k'}|e\rangle$. Phase shifts or ro-

tations of this state are accomplished by coupling the two levels with a pulse of appropriate length, Rabi frequency and detuning. The transformed state is then restored to the Rydberg basis. Thus multilevel transforms in the atom are possible with a timed sequence of laser pulses, without the need for multiple lasers to address the different Rydberg transitions. Moreover the fidelity of the gate operations compares favorably with that in an equivalent system of entangled two-level atoms [3].

For efficiently scalable quantum computing, we require conditional transforms on two entangled multilevel atoms. The method used in Ref. [3] is based on the linear ion trap scheme for binary quantum logic [15]. This scheme provides a means to evolve one two-level atom in the trap array conditional on the state of another two-level atom. Since the wave packet approach allows each basis amplitude in the atom to be addressed sequentially through low-lying energy levels, conditional transforms on other atoms can be carried out using the same methods as in the binary scheme. That is, conditional on a given wave packet state (vis à vis energy level) in the control atom, a d-dimensional transform is performed on the wave packet basis of the target atom using the methods outlined above.

The time taken to couple two atoms in this approach can be on the order of the atomic Kepler period, which permits a fast non-adiabatic coupling scheme. Also, the mean energy and number of Rydberg levels used depend ultimately on the ionization threshold imposed by external fields in the environment. We anticipate that neutral atom schemes that allow fast coupling times, as have been suggested recently [16], will provide a useful setting for multilevel quantum information applications.

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