# Time-dependent occupation numbers in reduced-density-matrix functional theory: Correlation-induced oscillations

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We prove that if the two-body terms in the equation of motion for the one-body reduced density matrix are approximated at each instant of time from ground-state functionals, the eigenvalues of the one-body reduced density matrix (occupation numbers) are time independent. This deficiency is related to the inability of such an approximation to account for relative phases that accumulate in the two-body reduced density matrix as time passes. We derive an exact differential equation giving the functional dependence of these phases in an interacting Landau-Zener model and study their behavior in short-time and long-time regimes. In the long-time regime, the occupation numbers display correlation-induced oscillations and the memory dependence assumes a simple form.

The effective single-particle scheme in reduced-density-matrix functional theory [1] (RDMFT) differs from the Kohn-Sham equations [2] of density functional theory and the Hartree-Fock equations in that essentially all orbitals have fractional ($0 < n_i < 1$) as opposed to integer occupation numbers. The freedom to occupy orbitals fractionally is helpful in correctly describing static correlation, a notoriously difficult problem in density functional theory. Static correlation is generally related to the multiconfigurational character of the wave function. Limiting oneself to integer occupation numbers amounts to trying to describe certain observables of a multiconfigurational state, such as energy or density, with only a single configuration (Slater determinant). As a consequence, the orbitals can lose any resemblance to the optimal orbitals for describing the wave function, the so-called *natural orbitals* [3]. In dynamical problems, the time dependence of the occupation numbers represents changes in the degree and character of correlation [4]. Changes in the occupation numbers have been shown to be crucial for describing double excitations [5–7].

In RDMFT, the wave function is interpreted as a functional of the one-body reduced density matrix (one-matrix) $\gamma(1, 1'; t) = \langle \Psi(t) | \hat{\psi}^\dagger(1') \hat{\psi}(1) | \Psi(t) \rangle$ ($1 = \mathbf{r}_1, \sigma_1$). The equation of motion is (in units $|e| = \hbar = m = c = 1$)

$$i\partial_t \hat{\gamma} = \left[ \frac{1}{2}(\hat{\mathbf{p}} - \hat{\mathbf{A}})^2 + \hat{v}, \hat{\gamma} \right] + \hat{u} \qquad (1)$$

where $\hat{v}$ and $\hat{\mathbf{A}}$ describe time-dependent external electromagnetic fields and

$$\langle 1 | \hat{u} | 1' \rangle = 2 \int d2 \left[ v_C(1, 2) - v_C(1', 2) \right] \Gamma(12, 1'2; t), \quad (2)$$

$\Gamma(12, 1'2'; t) = \frac{1}{2} \langle \Psi(t) | \hat{\psi}^\dagger(1') \hat{\psi}^\dagger(2') \hat{\psi}(2) \hat{\psi}(1) | \Psi(t) \rangle$ is the two-body reduced density matrix (two-matrix) and $v_C$ is the Coulomb potential. Equation (1) can be closed by interpreting the two-matrix as a functional of the one-matrix. In fact, it follows [8, 9] from the Runge-Gross

theorem [10], or its extension to include vector potentials [11, 12], that there exists an exact two-matrix functional $\Gamma([\gamma]; t)$. In general $\Gamma([\gamma]; t)$ has a functional dependence on $\gamma(t')$ for all $t' \leq t$. Instead of propagating the one-matrix directly, it is often more convenient to propagate its eigenfunctions and eigenvalues, called natural orbitals and occupation numbers, respectively, according to the equations [8, 13, 14]

$$i |\dot{\phi}_k\rangle = \left[ \frac{1}{2}(\hat{\mathbf{p}} - \hat{\mathbf{A}})^2 + \hat{v} + \hat{v}_{ee} \right] |\phi_k\rangle, \qquad (3)$$

$$\dot{n}_k = -i \langle \phi_k | \hat{u} | \phi_k \rangle = 4 \, \text{Im} \sum_{ijl} \Gamma_{ijkl} V_{klij} \qquad (4)$$

where the dot represents time derivative, $v_{ee,jk} = \langle \phi_j | \hat{v}_{ee} | \phi_k \rangle = u_{jk}/(n_k - n_j)$ ($j \neq k$), and $\Gamma_{ijkl}$ and $V_{ijkl}$ are the two-matrix and Coulomb integral, respectively, in the basis of natural orbitals.

In this letter, we report three fundamental results concerning the time dependence of the occupation numbers: (i) we prove that the occupation numbers are time independent when the exact functional $\Gamma([\gamma]; t)$ is approximated by the adiabatic extension of *any* ground-state (gs) functional $\Gamma[\gamma]$, (ii) for the generic crossing of two single-particle levels coupled by interactions, a generalization of the Landau-Zener (LZ) model, we find exact expressions for all the degrees of freedom of $\Gamma([\gamma]; t)$, and (iii) we identify oscillations in the occupation numbers with frequency of the order of the correlation energy. Result (i) was stated in Ref. 15 (see also Ref. 8); however, the arguments given to support the statement are incorrect [16]. Memory-dependent approximations for $\Gamma([\gamma]; t)$ are needed to capture the effects of nonadiabatic transitions on the occupation numbers, and (ii) and (iii) provide important exact results in an *interacting* LZ model.

If the external driving via $v(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ is slow, one might attempt an adiabatic extension approximation (AEA) in which the gs functional $\Gamma[\gamma]$ evaluated at the instantaneous $\gamma(t)$ is used in place of the functional $\Gamma([\gamma]; t)$ in Eqs. (3) and (4). However, it was realized [4, 8, 13] that

when the AEA is applied to the available approximate Hartree-Fock-type gs functionals, the occupation numbers remain constant in time because the right-hand-side of Eq. (4) vanishes. This left open the possibility that time-dependent occupation numbers could be obtained from a gs functional of a more general form [4, 8, 13].

One might suppose that neglecting the time dependence of the the occupation numbers would be a good approximation in the adiabatic regime, where indeed their time derivatives are very small. While this is often true, it is not always the case. Even external driving that is too slow to cause nonadiabatic transitions can lead to significant net changes in the occupation numbers if it acts for a long enough time. Therefore, the AEA is not a valid adiabatic approximation because it is inconsistent with the adiabatic theorem [17]. Since in the adiabatic regime the evolving wave function must remain close to the instantaneous ground state, an alternative adiabatic approximation was proposed [14], in which the orbitals satisfy Eq. (3) while the occupation numbers are obtained on-the-fly from the constrained minimization of the gs energy functional $E_v[\gamma]$ with $v = v(t)$. This approximation respects the adiabatic theorem and describes fairly well the lowest-order nonadiabatic effects.

In cases where the occupation numbers deviate greatly from their instantaneous gs values, it becomes preferable to propagate Eq. (4). Alternatively, one can step up in the hierarchy of equations of motion and propagate the two-matrix. Semiclassical propagation of the many-body density matrix has also been proposed [18] as a way to obtain time-dependent occupation numbers. With regard to the design of functionals $\Gamma([\gamma]; t)$ capable of changing the occupation numbers, it is important to know whether the failure of the AEA is due to the restrictive form of the gs functionals to which it was applied or whether it is inherent to the AEA itself. We shall now prove that the occupation numbers are *always* constant in the AEA.

Consider a system in its ground state at $t = t_0$ that experiences the external driving $v(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$ for $t \geq t_0$. If we exclude external driving that turns on discontinuously, then $\dot{\gamma}(t_0) = 0$ because the system is in a stationary state at $t = t_0$. This implies $|\dot{\phi}_k(t_0)\rangle = 0$ and $\dot{n}_k(t_0) = 0$. We can immediately conclude that $\dot{n}_k = 0$ for *all* time because within the AEA the right-hand side of Eq. (4) at time $t$ can be understood as an expression calculated for a system in a ground state with the one-matrix $\gamma(t)$ (provided $\gamma(t)$ remains ensemble $v$-representable). This expression must vanish since the ground state is a stationary state. In other words, in the AEA the right-hand side of Eq. (4) is an instantaneous functional of $\gamma$ by virtue of Gilbert's extension [1] of the Hohenberg-Kohn theorem; this functional is equal to the $\dot{n}_k$ of the unique gs density matrix corresponding to that $\gamma$; all such $\dot{n}_k$ vanish due to stationarity; hence, also the functional must vanish. Our assumption that the external driving does not turn on in a discontinuous manner

is consistent with the physically important case that the one-matrix is an analytic function of time.

Note that the above arguments would not be valid if the external driving $v(\mathbf{r}, t)$ or $\mathbf{A}(\mathbf{r}, t)$ were to appear explicitly in Eq. (4), as $\gamma(t)$ is generally the ground state of a system with different potentials, $v'(\mathbf{r})$ and $\mathbf{A}'(\mathbf{r})$, which would result in a mismatch. Accordingly, this line of argument does not apply to the orbital equation, revealing a dichotomy of the degrees of freedom that is a key feature of RDMFT. The occupation numbers are driven not by the external fields directly but by changes in the internal correlation of the system.

What is the gs $\Gamma[\gamma]$ missing? For two-electron singlet states, it has been shown [14] that the phases between the configurations that compose the wave function must differ from their gs values in order to obtain time-dependent occupation numbers in Eq. (4). Generally these relative configuration phases strongly influence phases in $\Gamma$. The AEA fails to generate time-dependent occupation numbers because, being based solely on the gs functional $\Gamma[\gamma]$, it cannot change the two-matrix phases away from their gs values. For two-electron singlet states, there is a one-to-one correspondence between the configuration phases and the phases in $\Gamma$. This is apparent from the Löwdin-Shull wave function [19]

$$|\Psi^{LS}\rangle = \frac{1}{\sqrt{2}} e^{-i\mu} \sum_k e^{-i2\zeta_k} \sqrt{n_k} \, |k\!\uparrow k\!\downarrow\rangle, \qquad (5)$$

where $|k\!\uparrow k\!\downarrow\rangle$ is the Slater determinant of $\phi_{k\uparrow}$ and $\phi_{k\downarrow}$ and we have made explicit the configuration phases $2\zeta_k$. The $\zeta_k$ influence the phases in $\Gamma$ as seen in the expression $\Gamma_{ijkl} = \frac{1}{2} e^{i2(\zeta_k - \zeta_i)} \sqrt{n_i n_k} \delta_{ij} \delta_{kl}$. We shall now study how the two-matrix phases evolve in time in a generic model.

*Interacting Landau-Zener model.*—We consider two interacting electrons occupying two single-particle levels whose bare energies cross linearly in time. We consider only the sector of singlet states, so the dimension of the relevant Hilbert subspace is three. The model is a generalization of the LZ problem and represents a typical *correlated* avoided crossing that one encounters in many-electron systems. Occupation numbers vary most rapidly near such avoided crossings. A many-electron system can be mapped onto this model by allowing effective time-dependent parameters. The Hamiltonian with the most general one-body and two-body interactions is

$$\hat{H} = \frac{1}{2}\vec{V} \cdot \hat{\vec{\sigma}} + \hat{U} + \hat{W}, \qquad (6)$$

where $\hat{\vec{\sigma}} = \sum_\sigma (\hat{c}_{1\sigma}^\dagger, \hat{c}_{2\sigma}^\dagger) \vec{\sigma} \begin{pmatrix} \hat{c}_{1\sigma} \\ \hat{c}_{2\sigma} \end{pmatrix}$, $\hat{U} = U_1 \hat{c}_{1\uparrow}^\dagger \hat{c}_{1\uparrow} \hat{c}_{1\downarrow}^\dagger \hat{c}_{1\downarrow} + U_2 \hat{c}_{2\uparrow}^\dagger \hat{c}_{2\uparrow} \hat{c}_{2\downarrow}^\dagger \hat{c}_{2\downarrow}$, and $\hat{W} = (W_1 - iW_2) c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow} + (W_1 + iW_2) c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger c_{1\downarrow} c_{1\uparrow}$. The spin-summed one-matrix in this model is simply a $2 \times 2$ Hermitian matrix $\gamma = I + \vec{\gamma} \cdot \vec{\sigma}$ with $\vec{\gamma} = A(\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ in spherical coordinates. The natural orbitals are

$\phi_a = (\cos(\theta/2)e^{-i\varphi/2}, \sin(\theta/2)e^{i\varphi/2})^T$ and $\phi_b = (-\sin(\theta/2)e^{-i\varphi/2}, \cos(\theta/2)e^{i\varphi/2})^T$ and have occupation numbers $n_a = 1 + A$ and $n_b = 1 - A$. Eqs. (3) and (4) become

$$i\dot{\phi}_k = \left(\frac{1}{2}\vec{V}\cdot\vec{\sigma} + v_{ee}\right)\phi_k \qquad (7)$$

$$\dot{A} = -\frac{i}{2}(u_{aa} - u_{bb}). \qquad (8)$$

In Eq. (7), $v_{ee}$ is the contribution of the two-body interactions $\hat{U}$ and $\hat{W}$ to the effective single-particle Hamiltonian. In the natural orbital basis, its off-diagonal elements are given by $v_{ee,ab} = -u_{ab}/2A$, while its diagonal elements are indeterminant and irrelevant because the phases of the natural orbitals are undefined. Direct calculation with a wave function of the form in Eq. (5) gives

$$u_{ab} = \overline{U}(1 + Be^{-i2\zeta})\sin\theta\cos\theta + \Delta U A \sin\theta$$
$$- |W|(1 + Be^{-i2\zeta})\sin\theta\cos\theta\cos(2\varphi - \omega)$$
$$- i|W|(1 - Be^{-i2\zeta})\sin\theta\sin(2\varphi - \omega), \qquad (9)$$

where $B = \sqrt{1 - A^2}$, $|W|e^{-i\omega} = W_1 - iW_2$, $\overline{U} = (U_1 + U_2)/2$, $\Delta U = (U_1 - U_2)/2$ and $\zeta = \zeta_a - \zeta_b$ is the relative configuration phase. The diagonal elements of $u$ enter in Eq. (8). We find $u_{aa} = -u_{bb}$ and

$$u_{aa} = -i\overline{U}B\sin^2\theta\sin 2\zeta - i2|W|B\cos\theta\sin(2\varphi - \omega)$$
$$\times \cos 2\zeta - i|W|B(1 + \cos^2\theta)\cos(2\varphi - \omega)\sin 2\zeta.$$

The dynamical equation for $\zeta$ can be readily obtained by transforming the Schrödinger equation to the basis $\{|a\uparrow a\downarrow\rangle, \frac{1}{\sqrt{2}}(|a\uparrow b\downarrow\rangle - |a\downarrow b\uparrow\rangle), |b\uparrow b\downarrow\rangle\}$. We find

$$\dot{\zeta} = \frac{1}{A}\vec{V}\cdot\vec{\gamma} + \frac{\overline{U}}{2}\frac{A}{B}\sin^2\theta\cos 2\zeta + \Delta U\cos\theta + \frac{|W|}{2}\frac{A}{B}$$
$$\times (1 + \cos^2\theta)\cos(2\varphi - \omega)\cos 2\zeta - |W|\frac{A}{B}\cos\theta$$
$$\times \sin(2\varphi - \omega)\sin 2\zeta - \dot{\varphi}\cos\theta. \qquad (10)$$

This can also be derived from the stationarity of the quantum action $S[\Psi] = \int dt\langle\Psi|H - i\partial_t|\Psi\rangle$ w.r.t. to $A$. The exact energy is $E[\Psi] = \vec{V}\cdot\vec{\gamma} + U[\Psi] + W[\Psi]$ with

$$U[\Psi] = \frac{\overline{U}}{2}(1 + \cos^2\theta) - \frac{\overline{U}}{2}B\sin^2\theta\cos 2\zeta + \Delta U A\cos\theta,$$

$$W[\Psi] = \frac{|W|}{2}\sin^2\theta\cos(2\varphi - \omega) + |W|B\cos\theta\sin(2\varphi - \omega)$$
$$\times \sin 2\zeta - \frac{|W|}{2}B(1 + \cos^2\theta)\cos(2\varphi - \omega)\cos 2\zeta.$$

and $i\int dt\langle\Psi|\dot{\Psi}\rangle = \int dt(\dot{\mu} + A\dot{\zeta} + A\dot{\varphi}\cos\theta)$. The gs Berry phase, $-i\int dt\langle\Psi_0|\dot{\Psi}_0\rangle = -\int dt A\dot{\varphi}\cos\theta$, depends only on the one-matrix variables $(A, \theta, \varphi)$. This expression gives a clear illustration of how interactions reduce the Berry phase with respect to its bare noninteracting value

$-\int dt\dot{\varphi}\cos\theta$ via the factor $A$ in the integrand. The one-matrix vector $\vec{\gamma}$ is similar to a pseudospin vector except its modulus $A$ is less than 1 due to electronic correlations.

Equations (7), (8) and (10) are a closed set of equations that describe the time evolution of $|\Psi\rangle$. In RDMFT, the configuration phase $\zeta$ is interpreted as a functional of $\gamma$—in the present case, the set of variables $(A, \theta, \varphi)$. Since for a fixed initial state the mapping $\vec{V}(t) \to \vec{\gamma}(t)$ is generally invertible, the memory-dependent functional $\zeta([\gamma];t)$ is given uniquely by the solution of Eq. (10). One possible adiabatic approximation is to set $\zeta$ to its instantaneous gs value on the right-hand side of Eq. (10). The first five terms are then seen to be $\partial E_v[\gamma]/\partial A$, and the last term comes from the gs Berry phase. In the case of linear-time external driving $\vec{V} = (V_1, 0, t/\tau)$, we now consider the short-time and long-time regimes of a system that starts in the ground state.

*Short-time regime.*—The stationary conditions imply $\dot{\gamma}(t_0) = 0$ and $\dot{\zeta}(t_0) = 0$. The lowest nonvanishing time-derivative at the initial time is $\ddot{\varphi}(t_0) = \dot{V}_3(t_0)$. This induces the following nonvanishing third time-derivatives:

$$\dddot{\varphi} = \ddot{\varphi}\Big[V_\perp\cot\theta\sin(\varphi - \varphi_V) + 2|W|\frac{B}{A}\cos(2\varphi - \omega)\sin 2\zeta$$
$$+ 2|W|\frac{1 + B\cos 2\zeta}{A}\cos\theta\sin(2\varphi - \omega)\Big],$$
$$\dddot{\theta} = -\ddot{\varphi}\Big[V_\perp\cos(\varphi - \varphi_V) + |W|\frac{B}{A}\sin 2\theta\sin(2\varphi - \omega)$$
$$\times \sin 2\zeta + 2|W|\frac{1 - B\cos 2\zeta}{A}\sin\theta\cos(2\varphi - \omega)\Big],$$
$$\dddot{\zeta} = -\ddot{\varphi}\Big[V_\perp\sin\theta\sin(\varphi - \varphi_V) + |W|\frac{A}{B}(1 + \cos^2\theta)$$
$$\times \sin(2\varphi - \omega)\cos 2\zeta + 2|W|\frac{A}{B}\cos\theta\cos(2\varphi - \omega)\sin 2\zeta\Big]$$
$$- \ddot{\varphi}\cos\theta,$$

where $V_\perp \equiv \sqrt{V_1^2 + V_2^2}$ and $\varphi_V \equiv \tan^{-1}(V_2/V_1)$. The lowest nonvanishing time-derivative of $A$ is $A^{(4)} = (\partial\dot{A}/\partial\theta)\,\dddot{\theta} + (\partial\dot{A}/\partial\varphi)\,\dddot{\varphi} + (\partial\dot{A}/\partial\zeta)\,\dddot{\zeta}$. The configuration phase and the occupation numbers change even more slowly if $|W| = 0$, for then the stationary condition $\partial E/\partial\varphi = 0$ implies $\varphi = \varphi_V + \pi$ so that $\dddot{\varphi} = \dddot{\zeta} = 0$ and $\partial\dot{A}/\partial\theta = 0$. Thus, the lowest nonvanishing time-derivative of $A$ is the fifth time-derivative, and the changes proceed via $\dot{V}_3 \to \ddot{\varphi} \to \dddot{\theta} \to \zeta^{(4)} \to A^{(5)}$.

*Long-time regime.*— For simplicity, we now consider the case $U_1 = U_2$ and $W = 0$. In the asymptotic limit $t \to \infty$, $\vec{\gamma}$ displays multiple oscillations with frequencies $\Omega_{ij} \equiv E_i - E_j$, where $E_i$ are the adiabatic energy levels. As the driving vector $\vec{V}$ diverges linearly as $t \to \infty$, the frequencies also diverge linearly. In contrast, the occupation numbers oscillate with the *constant* frequency $\Omega_{32} - \Omega_{21} = 2U$, as seen in Fig. (1). The exact asymptotic behavior of $A(t)$ is

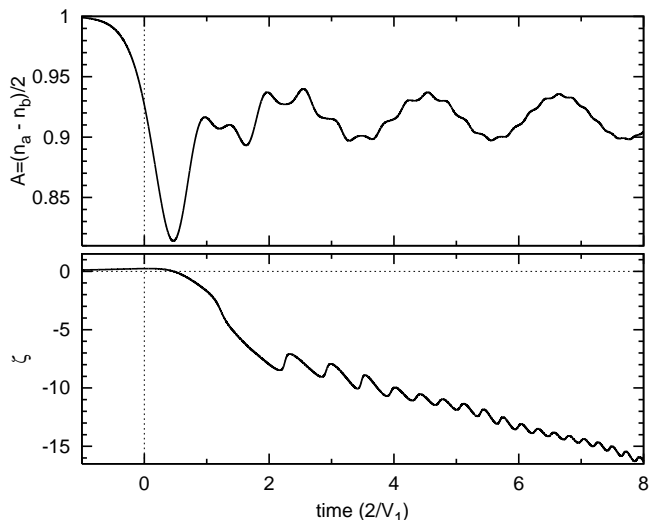$$A(t) = \sqrt{\overline{A}^2 + \Delta^2\cos\left[2Ut - (\Theta_{32} - \Theta_{21})\right]}, \qquad (11)$$

FIG. 1: Time dependence of $A$ and $\zeta$ for $|W| = 0$, $U_1 = U_2 = 3/2$, $t_0 = -4$ and linear-time driving $\vec{V} = (-2, 0, 4t)$.

where $\overline{A}^2 \equiv \gamma_{3,\infty}^2 + 2|c_2|^2(|c_1|^2+|c_3|^2)$, $\Delta^2 \equiv 4|c_1||c_2|^2|c_3|$, $\Theta_{ij} \equiv \mathrm{Arg}(c_i/c_j)$ and $c_i$ are the coefficients in the expansion $|\Psi\rangle = \sum_i c_i \exp[-i\int dt(E_i - i\langle\Phi_i|\partial_t\Phi_i\rangle)]|\Phi_i\rangle$ over the adiabatic eigenstates $|\Phi_i\rangle$. We have also defined $\gamma_{3,\infty} \equiv \gamma_3(\infty) = const$. As $t \to \infty$, $\varphi$ has a component that grows quadratically in time, i.e., $\varphi \sim t^2/2\tau$, which implies $\vec{\gamma}$ rotates more and more rapidly around the south pole of the Bloch sphere. Hence, any terms in the dynamical equations containing periodic functions of $\varphi$ quickly average to zero. Dropping such terms, we find

$$\dot{A} = -UB\sin^2\theta\sin 2\zeta \tag{12}$$

$$\dot{\zeta} = -U\frac{1 + B\cos\zeta}{A}\cos^2\theta + \frac{U}{2}\frac{A}{B}\sin^2\theta\cos 2\zeta. \tag{13}$$

Although $\theta$ appears in these equations, it can be eliminated in favor of $A$ by means of the asymptotic relationship $\gamma_{3,\infty} = A\cos\theta$. Therefore, the equations for $A$ and $\zeta$ are decoupled from those for the orbital variables $\theta$ and $\varphi$. Eqs. (12) and (13) can be expressed in the form of Hamilton's canonical equations,

$$\dot{A} = -\frac{\partial U[\Psi]}{\partial \zeta} \tag{14}$$

$$\dot{\zeta} = \frac{\partial U[\Psi]}{\partial A}, \tag{15}$$

where $A$ and $\zeta$ appear as conjugate variables. Eqs. (14) and (15) are integrable because $U_\infty \equiv \lim_{t\to\infty} U[\Psi]$ is a conserved quantity. Integrability has important consequences for memory dependence. Since $U_\infty$ is a constant of the motion, it can be expressed as a function of $A$, $\zeta$ and $\gamma_{3,\infty}$. Hence, there is an *instantaneous* relationship between $A$ and $\zeta$ in the asymptotic limit. It is, explicitly,

$$\cos 2\zeta = \frac{2A^2\left(1 - \frac{U_\infty}{U}\right) - (A^2 - \gamma_{3,\infty}^2)}{\sqrt{1 - A^2}(A^2 - \gamma_{3,\infty}^2)}. \tag{16}$$

The constant $\gamma_{3,\infty}$ contains information about the non-adiabatic transitions that occurred near $t = 0$. Therefore, the $\gamma$-dependence of the functional $\zeta([\gamma]; t)$ separates into two distinct types: (i) an ultra-local (instantaneous) dependence on $A(t)$ and (ii) an ultra-nonlocal dependence on $\gamma(t)$ near $t = 0$ that enters only through the constant $\gamma_{3,\infty}$. In the asymptotic regime, the $\gamma_{3,\infty}$ dependence can be treated as initial-state dependence. If Eqs. (14) and (15) were nonintegrable, we expect the functional $\zeta([\gamma]; t)$ would have more complex memory dependence.

The asymptotic $\zeta(t)$ described by Eqs. (16) and (11) is a linearly decreasing function with superimposed nonlinear oscillations. The slope $\sim -U$ corresponds to the frequency of the correlation-induced oscillations in $A(t)$, as seen in Fig. (1). The sudden positive jumps in $\zeta$ are due to the term $\dot{\varphi}\cos\theta$, which comes from the Berry phase. It is strongly peaked because when $\vec{\gamma}$ passes close to the south pole, $\dot{\varphi}$ is large. The south pole ($\gamma_3 = -1$) corresponds to full occupancy ($n_{i\uparrow} + n_{i\downarrow} = 2$) of site 2.

*Conclusions.*—We have proved that approximations for $\Gamma([\gamma]; t)$ going beyond the adiabatic extension of the gs $\Gamma[\gamma]$ are required to achieve time-dependent occupation numbers in the self-consistent propagation of the one-matrix equation of motion. The gs $\Gamma[\gamma]$ lacks dynamical phases present in the exact $\Gamma([\gamma]; t)$. The correlated LZ problem studied here provides important insights into the behavior of these phases in many-body systems.

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