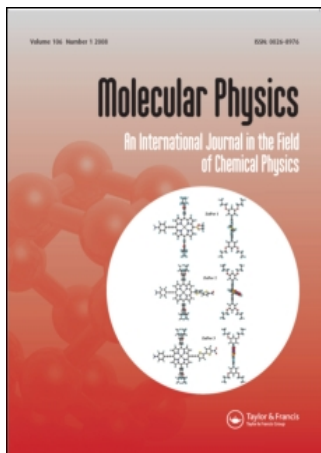


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#### Adiabatic molecular dynamics: two-body and many-body aspects

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## RESEARCH ARTICLE

### Adiabatic molecular dynamics: two-body and many-body aspects

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We compare various types of adiabatic dynamics that occur during atomic collisions and molecular dynamics. Born–Oppenheimer and non-adiabatic effects in molecular dynamics are contrasted with the time-dependent Landau–Zener transition problem for transitions that occur when a parameter in the Hamiltonian is varied slowly, and these are contrasted with the coherent many-body transitions that occur for a degenerate gas of atoms when an external parameter is tuned slowly near a Feshbach resonance to create loosely bound molecules. Analysis of an adiabatic sweep through a Feshbach resonance in a quantum gas of fermionic atoms shows that the dependence of the remaining atomic fraction on the sweep rate  $\alpha$  varies from exponential Landau–Zener behaviour for a single pair of particles to a power-law dependence for large particle number  $N$ .

**Keywords:** adiabatic dynamics; Landau–Zener transition; coherent many-body effects; Feshbach resonance

#### 1. Introduction: two-body collision dynamics

Numerous phenomena in atomic, molecular and optical physics are naturally described in an adiabatic formulation wherein the internal basis states are parametrically dependent upon a relative coordinate [1–7], or upon time [8–16], which slowly varies. Adiabatic here means ‘slow’, and therefore is quite distinct from adiabatic in the thermodynamic sense [17,18].

In the adiabatic representation of collisions between atoms, one takes the full wave function  $\Psi(r, R)$  and represents it in the form of a product of an internal wave function for the electrons,  $\phi(r, R)$ , which depends parametrically on the relative coordinate  $R$  and a relative nuclear-coordinate wave function  $F(R)$  [2,3]:

$$\Psi_j(r, R) = \sum_i \phi_i(r, R) F_{i,j}(R). \quad (1)$$

Here,  $r$  represents the internal set of coordinates, i.e. the electronic coordinates. The Schrödinger equation at energy  $E$  for the nuclear wave function  $\mathbf{F}(R)$  is obtained by taking matrix elements with the internal wave functions  $\phi_i(r, R)$  over the internal degrees of freedom  $r$  of the full Schrödinger equation,  $(H_N + H_{el})\Psi = E\Psi$ , where  $H_N$  and  $H_{el}$  are the nuclear and electronic Hamiltonian, respectively. In atomic units we obtain [3]

$$\left[ -\frac{1}{2\mu} \frac{d^2}{dR^2} \mathbf{I} + \mathbf{U}(R) - \frac{1}{2\mu} \left( 2\mathbf{A} \frac{d}{dR} + \mathbf{B} \right) \right] \mathbf{F} = E\mathbf{F}, \quad (2)$$

where  $\mathbf{A}$  and  $\mathbf{B}$  are the first and second derivative coupling matrices and  $\mathbf{U}(R)$  is the potential matrix obtained by solving the electronic problem at inter-nuclear coordinate  $R$ . The matrix  $\mathbf{A}$  is anti-hermitian and is given by

$$A_{ij}(R) = \left\langle \phi_i(r, R) \left| \frac{d}{dR} \right| \phi_j(r, R) \right\rangle_r, \quad (3)$$

and the second derivative coupling matrix  $\mathbf{B}$  is

$$B_{ij}(R) = \left\langle \phi_i(r, R) \left| \frac{d^2}{dR^2} \right| \phi_j(r, R) \right\rangle_r. \quad (4)$$

The second derivative term  $\mathbf{B}$  is neither Hermitian nor anti-Hermitian. Nevertheless,  $2\mathbf{A}(R)(d/dR) + \mathbf{B}(R)$  is Hermitian. The terms in Equation (2) involving  $\mathbf{A}$  and  $\mathbf{B}$  are usually referred to as non-adiabatic correction terms. In this representation, the radial derivative coupling terms coming from the nuclear angular momentum terms are not explicitly shown, i.e. they are buried in the matrix  $\mathbf{U}$ . In this language, the adiabatic Born–Oppenheimer approximation corresponds to neglecting the first and second derivative coupling terms, and the non-adiabatic calculation is carried out by including them. An identical formalism can be used for treating electronic conductance in mesoscopic waveguide systems [4], where the deformations of the waveguide (constrictions and openings of the waveguide down the channel) are modeled through

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the dependence of the mode functions  $\phi_i(r,R)$  on the orthogonal degrees of freedom of the waveguide  $R$ , and  $r$  is the coordinate along the waveguide axis (i.e. in the language of chemical reaction dynamics, the reaction coordinate).

Another aspect of adiabaticity, and a measure of non-adiabaticity, is manifest in the time-dependent quantum mechanical paradigm called the Landau–Zener (LZ) problem. This refers to a problem first solved by Landau and Zener in 1932 [8], wherein a two-level system whose energy difference varies linearly in time with a rate of change  $\alpha$  is coupled by a constant coupling matrix element  $V$ . The time-dependent  $2 \times 2$  Hamiltonian matrix can be written as

$$H(t) = \begin{pmatrix} \epsilon_1 & V \\ V & \epsilon_2 + \alpha t \end{pmatrix}. \quad (5)$$

We need to find the transition probability of finding the system in one state, say state 2 as  $t \rightarrow \infty$ , if it was in state 1 as  $t \rightarrow -\infty$ . For infinitely slow variation of the rate of energy difference,  $\alpha = 0$ , no transition between levels takes place. For finite  $\alpha$ , the transition probability  $P_{LZ}$  depends exponentially on the inverse rate of change of the energy difference [8]:

$$P_{LZ} = \exp\left(-\frac{2\pi V^2}{\alpha}\right). \quad (6)$$

This expression is not analytic in the rate of energy change  $\alpha$ , hence a perturbation expansion in  $\alpha$  cannot yield this result.

An interesting twist on the Landau–Zener problem involves transitions in multistate curve crossing problems. These may be represented intuitively as a sequence of two-state crossings and avoided crossings. In the absence of turning points near the crossings, one would expect that the crossings should occur in the causal ordering of the crossing points along the direction of motion. It is, however, known from quantum close-coupling calculations that certain *counterintuitive* transitions may also be allowed [7,19,20], in which the causal arrangement may be broken, letting the second crossing point precede the first one with respect to the direction of motion. Such transitions, shown as the dashed curve in Figure 1, are generally forbidden in analytical semiclassical theories of multistate curve crossing, but can be incorporated with special care [7].

Landau–Zener models [8] can also be used to describe collisions of ground and excited laser cooled alkali atoms in the presence of near-resonant light when spontaneous emission or fine-structure changing collisions complicate the collision process [5,6]. Typically, these collisions lead to loss of atoms from

traps when the excited state  $e$  decays due to radiative or fine-structure-changing processes to a loss channel  $p$ . The Landau–Zener models only begin to fail at low temperatures, e.g. less than or nearly equal to  $T = 1, \mu\text{K}$ , and at large intensities [5]. The probability of exiting on the loss channel  $p$  when one starts at large distances in the ground state channel  $g$  is given by

$$P_p = |S_{gp}|^2 = P_{ep}(R_{in})J_e(R_{in}), \quad (7)$$

where the probability  $P_{ep} = |S_{ep}|^2$  measures the quantum probability of the  $e \rightarrow p$  inner zone process due to the inner curve-crossing process,  $R_{in}$  is the location of this inner zone curve crossing, and the quantum flux  $J_e(R_{in})$  is the quantum mechanical probability of reaching the inner zone on the excited state  $e$ , i.e. of getting to the crossing point  $R_{in}$  on the excited state  $e$ .

Here, we shall explore the generalisation of the Landau–Zener problem to many-body dynamics. We shall do so within the context of a problem of production of molecules or Cooper-pairs, from a gas of degenerate fermionic atoms having two spin states equally populated, by slowly changing the magnetic field strength in the region near a Feshbach resonance. When the atomic gas is degenerate, the collisions that occur near the Feshbach resonance cannot be viewed as collisions of individual atoms, two-at-a-time, to form a molecule, but the atomic collisions in the gas are collective. As a result, the nature of the slow time-dependence changes from the two-body Landau–Zener type of process to a collective behaviour having a power law rate, rather than an exponential rate behaviour.

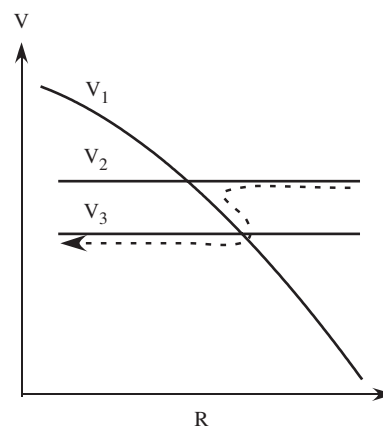


Figure 1. Schematic of a counterintuitive crossing of potentials. Transitions in such an arrangement are usually modeled as a sequence of two Landau–Zener crossings, but this is not adequate to describe the counterintuitive crossing. An analytic treatment of such crossings has been developed [7].

Algebraic approaches to quantum scattering have been pioneered by Levine and colleagues [21].

## 2. Many-body dynamics

We consider the collisionless, single bosonic mode Hamiltonian [22–27] for a degenerate gas of spin-up and spin-down fermions which can associate with a loosely bound molecular state whose energy varies with time because of the time-dependent sweep of an external magnetic field about values close to the Feshbach resonance field,

$$H = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \mathcal{E}(t) b_0^\dagger b_0 + g \left( \sum_{\mathbf{k}} c_{\mathbf{k},\uparrow} c_{-\mathbf{k},\downarrow} b_0^\dagger + H.c. \right), \quad (8)$$

where  $\epsilon_k = \hbar^2 k^2 / 2m$  is the kinetic energy of a fermionic atom with mass  $m$ , and  $g$  is the atom–molecule coupling strength. The molecular energy  $\mathcal{E}(t) = \alpha t$  is linearly swept at a rate  $\alpha$  through resonance to induce adiabatic conversion of fermionic atoms to Bose molecules. The annihilation operators for the atoms,  $c_{k,\sigma}$ , obey fermionic anticommutation relations, whereas the molecule annihilation operator  $b_0$  obeys a bosonic commutation relation.

The adiabatic conversion efficiency is insensitive to the details of the atomic dispersion provided that all atomic levels are swept through. Figure 2 shows exact numerical results for the adiabatic conversion of five atom pairs into molecules, for different values of the atomic level spacing (and hence of the Fermi energy  $E_F$ ). It is evident that, while the exact dynamics depends on  $E_F$ , levels are sequentially crossed, leading to the same final efficiency regardless of the atomic motional timescale. In particular, in the limit as  $\alpha \rightarrow 0$  it is possible to convert *all* atom pairs into molecules.

Since the exact energies  $\epsilon_k$  do not affect the final fraction of molecules, we use a degenerate model [26,27], with  $\epsilon_k = \epsilon$  for all  $\mathbf{k}$ . We define the operators [27,28]:

$$\mathcal{J}_- = \frac{b_0^\dagger \sum_{\mathbf{k}} c_{\mathbf{k},\uparrow} c_{-\mathbf{k},\downarrow}}{(N/2)^{3/2}}, \quad \mathcal{J}_+ = \frac{\sum_{\mathbf{k}} c_{-\mathbf{k},\downarrow}^\dagger c_{\mathbf{k},\uparrow}^\dagger b_0}{(N/2)^{3/2}}$$

$$\mathcal{J}_z = \frac{\sum_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma} - 2b_0^\dagger b_0}{N} \quad (9)$$

where  $N = 2b_0^\dagger b_0 + \sum_{k,\sigma} c_{k,\sigma}^\dagger c_{k,\sigma}$  is the conserved total number of particles. It is important to note that  $\mathcal{J}_-, \mathcal{J}_+, \mathcal{J}_z$  do not span  $SU(2)$  as  $[\mathcal{J}_+, \mathcal{J}_-]$  is a quadratic polynomial in  $\mathcal{J}_z$ . We also define  $\mathcal{J}_x = \mathcal{J}_+ + \mathcal{J}_-$  and  $\mathcal{J}_y = -i(\mathcal{J}_+ - \mathcal{J}_-)$ . Up to a  $c$ -number term, Hamiltonian (8) takes the form

$$H = \frac{N}{2} \left( \Delta(t) \mathcal{J}_z + g \sqrt{\frac{N}{2}} \mathcal{J}_x \right), \quad (10)$$

where  $\Delta(t) = 2\epsilon - \mathcal{E}(t)$ . Defining a rescaled time  $\tau = \sqrt{N}gt$ , we obtain the Heisenberg equations of motion for the association of a quantum-degenerate gas of fermions,

$$\frac{d}{d\tau} \mathcal{J}_x = \delta(\tau) \mathcal{J}_y,$$

$$\frac{d}{d\tau} \mathcal{J}_y = -\delta(\tau) \mathcal{J}_x + \frac{3\sqrt{2}}{4} (\mathcal{J}_z - 1)$$

$$\left( \mathcal{J}_z + \frac{1}{3} \right) - \frac{\sqrt{2}}{N} (1 + \mathcal{J}_z),$$

$$\frac{d}{d\tau} \mathcal{J}_z = \sqrt{2} \mathcal{J}_y, \quad (11)$$

which depend on the single parameter  $\delta(\tau) = \Delta(t) / \sqrt{N}g = (\alpha/g^2 N)\tau$ . We note parenthetically that precisely the same set of equations, with  $\mathcal{J}\mathcal{J}_z \rightarrow -\mathcal{J}\mathcal{J}_z$  and  $g \rightarrow g/2$ , is obtained for a two-

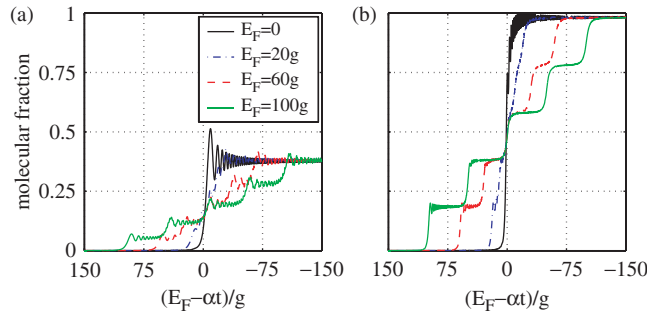


Figure 2. Many-body collective dynamics of adiabatic passage from a fermionic atomic gas into a molecular BEC for five pairs of fermionic atoms. (a) Sweep rate  $\alpha = 2g^2 N$ , (b) Sweep rate  $\alpha = g^2 N/4$ . Overall efficiency is independent of atomic dispersion in both (a) and (b).

mode atom–molecule BEC [28], providing another perspective on the recently observed mapping between the two systems [26,27].

The mean-field limit of Equations (11) is obtained by replacing  $\mathcal{J}_x, \mathcal{J}_y$ , and  $\mathcal{J}_z$  by their expectation values  $u, v$ , and  $w$ , which correspond to the real and imaginary parts of the atom–molecule coherence and the atom–molecule population imbalance, respectively, and omitting the quantum noise term  $\sqrt{2}(1 + \mathcal{J}_z)/N$ . In this limit, the equations depict the motion of a generalised Bloch vector on a two-dimensional surface, determined by the conservation law

$$u^2 + v^2 = \frac{1}{2}(w-1)^2(w+1). \quad (12)$$

Hamiltonian (10) is then replaced by the classical form

$$H(w, \theta; \Delta) = \frac{gN^{3/2}}{2} \left( \delta w + \sqrt{(1+w)(1-w)^2 \cos \theta} \right), \quad (13)$$

with  $\theta = \arctan(v/u)$ .

The atom–molecule adiabatic passage and the degree of non-adiabaticity can be ascertained using the method published previously [29]. The eigenvalues of the atom–molecule system at any given value of  $\delta$  correspond to the fixed points  $(u_0, v_0, w_0)$  of the classical Hamiltonian (13) or the mean-field limit of Equations (11):

$$v_0 = 0, \quad \frac{\sqrt{2}}{4}(w_0 - 1)(3w_0 + 1) = \delta u_0. \quad (14)$$

The number of fixed points depends on the parameter  $\delta$ . The point  $u_0 = v_0 = 0, w_0 = 1$  is stationary for any value of  $\delta$ . Using Equations (12) and (14), other fixed points satisfy

$$\frac{(3w_0 + 1)^2}{4(w_0 + 1)} = \delta^2. \quad (15)$$

For sufficiently large detuning,  $|\delta| > \sqrt{2}$ , Equation (15) has only one solution in the range  $-1 \leq w_0 \leq 1$ . Therefore, there are only two (elliptic) fixed points, corresponding to the solution of Equation (15), and  $(u, v, w) = (0, 0, 1)$ . As the detuning is changed, the first fixed point smoothly moves from all-molecules towards the atomic mode. At detuning  $\delta = -\sqrt{2}$  a homoclinic orbit appears through the point  $(0, 0, 1)$  which bifurcates into an unstable (hyperbolic) fixed point remaining on the atomic mode, and an elliptic fixed point which starts moving towards the molecular mode. Consequently, in the regime  $|\delta| < \sqrt{2}$  there are two elliptic fixed points and one hyperbolic fixed point, corresponding to the unstable all-atoms mode. Another crossing occurs at  $\delta = \sqrt{2}$  when the fixed

point which started near the molecular mode coalesces with the all-atoms mode. The frequency of small periodic orbits around the fixed points,  $\Omega_0$ , is found by linearization of the dynamical equations (11) about  $(u_0, v_0, w_0)$  and using (15) to obtain

$$\frac{\Omega_0}{g\sqrt{N}} = \sqrt{\delta^2 + (1 - 3w_0)} = \sqrt{\frac{(1 - w_0)(3w_0 + 5)}{4(w_0 + 1)}}. \quad (16)$$

Hence, for  $|\delta| < \sqrt{2}$  the period of the homoclinic trajectory beginning at  $(0, 0, 1)$  diverges.

Transforming  $w, \theta$  into action-angle variables  $I, \phi$ , the non-adiabatic probability  $\Gamma$  at any finite sweep rate  $\alpha$  is related to the action  $I$  accumulated during the sweep [8,29,30],

$$\Gamma^2 = \frac{\Delta I}{2} = \frac{1}{2} \int_{-\infty}^{\infty} R(I, \phi) \dot{\Delta} \frac{d\phi}{\dot{\phi}}, \quad (17)$$

where  $R(I, \phi)$  is related to the generating function of the canonical transformation  $w, \theta \rightarrow I, \phi$ . We note that, unlike the linear [8] or Josephson [29,30] case, where the tunneling probability is linearly proportional to the action increment  $\Delta I$ , our choice of variables (9) causes the atomic population at the end of the sweep (and hence,  $\Gamma$ ) to be proportional to the *square root* of  $\Delta I$  (since  $u^2(t_f) + v^2(t_f) \propto |\sum_{\mathbf{k}, \sigma} n_{\mathbf{k}, \sigma}(t_f)|^2$ , where  $n_{\mathbf{k}, \sigma}(t_f)$  is the population in state  $|\mathbf{k}, \sigma\rangle$  at the final time  $t_f$ ). Equation (17) depicts the familiar rule that in order to attain adiabaticity, the rate of change of the adiabatic fixed points through the variation of the adiabatic parameter  $\Delta$ ,  $R(I, \phi) \dot{\Delta}$ , should be slow with respect to the characteristic precession frequency  $\dot{\phi} = \Omega_0$  about these stationary vectors. For an adiabatic process where  $\dot{\Delta}/\dot{\phi} \rightarrow 0$  the action (which is proportional to the surface area enclosed within the periodic orbit) is an adiabatic invariant, so a zero-action elliptic fixed point evolves into a similar point trajectory. Action is accumulated mainly in the vicinity of singularities where  $\dot{\phi} = \Omega_0 \rightarrow 0$ . For linear adiabatic passage [8], such singular points lie exclusively off the real axis, leading to exponential Landau–Zener (LZ) transition probabilities. However, when nonlinearities are dominant, as in the Mott-insulating Josephson case [29,30] and our case, there are real singularities, leading to power-law dependence of the transfer efficiency on the sweep rate.

For atom–molecule conversion, a real singularity of the integrand in (17) exists at  $w_0 = 1$ , where the frequency vanishes as  $\Omega_0 \approx g\sqrt{N}(1 - w_0)$ , as is clear from (16). Hence, most of the non-adiabatic correction is accumulated in the vicinity of this point (all-atoms for fermions and all-molecules for bosons). Differentiating Equation (15) with respect to  $t$ , we

find that the response of the fixed-point velocity to a linear sweep rate is given by

$$\dot{w}_0 = \frac{4\alpha}{g\sqrt{N}} \frac{(w_0 + 1)^{3/2}}{3w_0 + 5}. \quad (18)$$

We can now find the action-angle variable  $\phi$  in terms of  $w_0$ :  $\phi = \int \dot{\phi} dt = \int \Omega_0 (dw_0/w_0)$ . In the vicinity of the singularity we have  $\Omega_0 \approx g\sqrt{N}(1-w_0)$  and  $\dot{w}_0 \approx \sqrt{2}\alpha/g\sqrt{N}$ , resulting in

$$\phi = \frac{g^2 N \sqrt{2}}{\alpha^3} (1-w_0)^{3/2}. \quad (19)$$

Using Equation (19), we finally find that, near the singularity,  $\dot{\phi} = \Omega_0 \approx g\sqrt{N}(1-w_0)$  is given in terms of  $\phi$  as

$$\dot{\phi} = \left(3\sqrt{\frac{N}{2}}g\alpha\right)^{1/3} \phi^{1/3}. \quad (20)$$

Substituting (20) and  $\dot{\Delta} = \alpha$  into Equation (17) we find that the non-adiabatic correction depends on  $\alpha$  as

$$\Gamma \propto \alpha^{1/3}. \quad (21)$$

So far, we have neglected the effect of quantum fluctuations, which are partially accounted for by the source term  $(\sqrt{2}/N)(1 + \mathcal{J}_z)$  in Equations (11). As a result, we found that  $\dot{w}_0$  does not vanish as  $w_0$  approaches 1. Consequently, the remaining atomic population is expected to scale as the cubic root of the sweep rate if the initial average molecular fraction is larger than the quantum noise. However, starting purely with fermion atoms (or with molecules made of bosonic atoms), fluctuations will initially dominate the conversion process. Equation (15) should then be replaced by

$$\delta = \frac{2}{\sqrt{w_0 + 1}} \left( \frac{3w_0 + 1}{4} - \frac{w_0 + 1}{N(w_0 - 1)} \right), \quad (22)$$

demonstrating that our previous treatment around  $w_0 = 1$  is only valid provided that  $|w_0(t_i) - 1| \gg 1/N$ . For a smaller initial molecular population, Equation (18) should be replaced by

$$\dot{w}_0 = \frac{\alpha}{g\sqrt{N}} \left/ \left[ \frac{3w_0 + 5}{4(w_0 + 1)^{3/2}} + \frac{w_0 + 3}{N(w_0 + 1)^{1/2}(w_0 - 1)^2} \right] \right. \quad (23)$$

Hence, in the vicinity of  $w_0 = 1$  the eigenvector velocity in the  $w$  direction vanishes as  $\dot{w}_0 = (\sqrt{N}\alpha/g\sqrt{8})(w_0 - 1)^2$ . The characteristic frequency  $\dot{\phi}$  is now proportional to  $(\alpha\phi)^{-1}$  instead of Equation (20) so that  $\Delta I \propto \alpha^2$ , and [31,32]

$$\Gamma \propto \alpha. \quad (24)$$

Equations (24) and (21) constitute the main results of this work. We predict that the remnant atomic fraction in adiabatic Feshbach sweep experiments will scale as a power-law with sweep rate due to the curve crossing in the nonlinear case. The dependence is expected to be linear if the initial molecular population is below the quantum-noise level (i.e. when  $1 - w_0(t_i) \ll 1/N$ ), and cubic-root when fluctuations can be neglected (i.e. for  $1 - w_0(t_i) \gg 1/N$ ). We note that a similar linear dependence was predicted for adiabatic passage from bosonic atoms into a molecular BEC [31].

The analytical predictions illustrated above are confirmed by numerical simulations. Figure 3 shows  $\Gamma$  versus dimensionless inverse sweep rate  $g^2/\alpha N$ . Exact many-body numerical calculations for particle numbers in the range  $2 \leq N \leq 800$ , carried out using published methodology [26], are compared with a mean-field curve (solid green line), computed numerically from the mean-field limit of Equations (11). The log-log plot highlights the power-law dependence, obtained in the slow ramp regime  $\alpha < g^2 N$ , whereas the log-linear insert plot demonstrates exponential behaviour (for  $N=2$ ). For a single pair of particles,  $N=2$ , the quantum association problem is formally identical to the linear LZ paradigm, leading to an exponential dependence of  $\Gamma$  on sweep rate. However, as the number of particles increases, many-body effects come into play, and there is a smooth transition to a power-law behaviour in the slow ramp regime  $\alpha < g^2 N$ . We note that this is precisely the regime where Equation (17) can be used to estimate  $\Delta I$  and  $\Gamma$  [8]. The many-body calculations converge to the mean-field limit, corresponding to a linear dependence of  $\Gamma$  on  $\alpha$ , as predicted in Equation (24).

Equation (17) reflects our discussion on characteristic timescales. In order to attain adiabaticity, the rate of change of the adiabatic fixed points through the variation of the adiabatic parameter  $\Delta$ ,  $R(I, \phi) \dot{\Delta}$ , should be slow with respect to the characteristic precession frequency  $\dot{\phi} = \Omega_0$  about these stationary vectors. The action increment is proportional to the ratio of these two timescales.

As long as  $\dot{\phi}$  does not vanish, the accumulated action can be minimised by decreasing  $\dot{\Delta}$ . For a perfectly adiabatic process where  $\dot{\Delta}/\dot{\phi} \rightarrow 0$ , the action is an adiabatic invariant, so that a zero-action elliptic fixed point evolves into a similar point trajectory. For finite sweep rate, the LZ prescription [8] evaluates the integral in (17) by integration in the complex plain, over the contour of Figure 4, noting that the main contributions will come

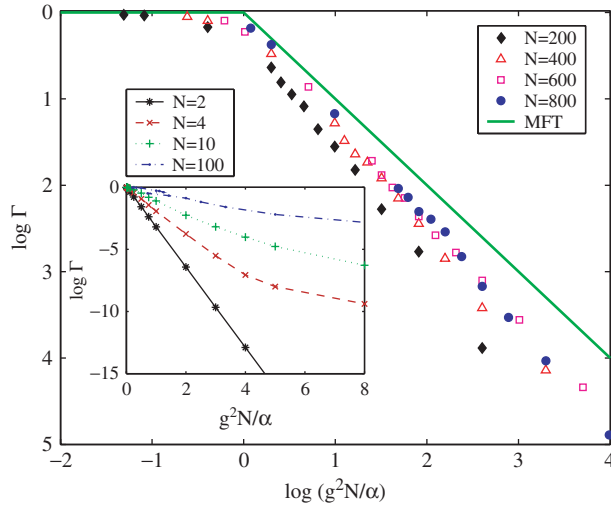


Figure 3. Many-body calculations for the fraction of remnant atoms,  $\Gamma$ , versus dimensionless inverse sweep rate for various particle numbers in the range  $N = 2$ –800. The many-body results for a large number of particles converge to the mean-field results (solid green line) of Figure 5.

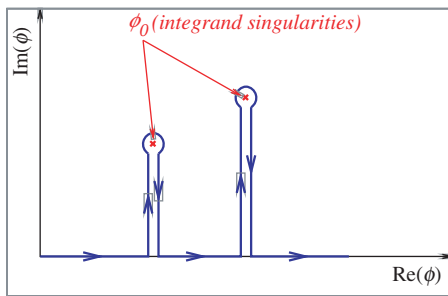


Figure 4. Contour of integration in Landau-Zener theory, for calculating the integral in Equation (17). All singularities lie off the real axis for the standard two-body Landau-Zener transition. Here, the singularities lie on the real axis.

from singular points, where  $\dot{\phi}$  approaches zero and the integrand diverges. Since for a linear LZ system there are no instabilities, all such singularities are guaranteed to lie off the real axis, leading to exponentially small LZ transition probabilities.

The situation changes for nonlinear systems, where instabilities arise. We have shown that for the atom-molecule system with fermion atoms, the all-atoms mode becomes unstable to association when the detuning hits the critical value of  $\delta_c = \sqrt{2}$ . From Equation (16) it is clear that the characteristic frequency  $\dot{\phi} = \Omega_0$  vanishes near  $w_0 = 1$ . Consequently, there are singular points of the integrand in (17) lying on the real axis. The poles on the real axis lead to a power-law dependence of the transfer efficiency on the sweep rate.

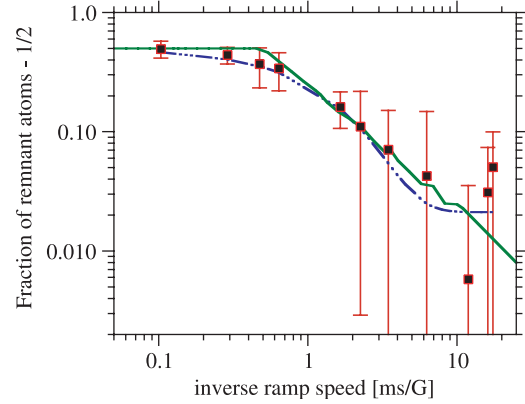


Figure 5. Fraction of remnant atoms,  $\Gamma$ , versus inverse ramp speed  $1/\dot{B}$  across the 543G resonance in a two-component Fermi gas of  $^6\text{Li}$ . The experimental data [34] (black squares), which saturates at a remnant of  $1/2$  [33], and the mean-field calculations (green solid curve) obey a linear dependence on sweep rate beyond  $0.5\text{ms/G}$ .  $g^2/\alpha N$  is multiplied by  $0.5\text{ms/G}$  to scale the abscissa for the calculated results. Also shown as a dashed blue curve is the best exponential fit to the data,  $\Gamma = 0.479 \exp(-\alpha/1.3) + 0.521$ .

### 3. Comparison with experiment

We compare our mean-field numerical calculation with published experimental data [34] on the narrow Feshbach resonance in Figure 5. The theory agrees very well with the experiment. However, since an equally good exponential fit can be found [34], as shown in Figure 5 (dashed line), the current experimental data does not serve to determine which of the alternative theories is more appropriate. We have obtained similar agreement with experimental data [35] on the  $^{40}\text{K}$  Feshbach resonance, but data scatter and error bars are again too large to conclusively resolve power-laws from exponentials. Further precise experimental data for slow ramp speeds and different particle numbers will be required to verify or to refute our theory.

### 4. Summary and conclusion

The process by which atoms go to molecules in a degenerate gas of fermions containing spin-up and spin-down states as a magnetic field is slowly varied with time near a Feshbach resonance corresponds to a special case of a quantum phase transition. A quantum phase transition is a qualitative change in the ground state of a system as a result of a small variation of an external parameter, e.g. a magnetic field. Ideally, this phase transition occurs at zero temperature, in contrast to thermodynamic

phase transitions. It leads to the creation of excitations whose density and scaling with the rate of change of the external parameter is described very generally by Kibble–Zurek theory [36]. Our theoretical model of the Feshbach resonance association process is a special case of this mechanism. Here, we have shown that many-body effects can play a significant role in the atom–molecule conversion process for degenerate fermionic atomic gases, modifying the Landau–Zener exponential dependence on sweep rate to a power-law dependence. This is but one special case of a zero-temperature many-body phase transition. The collective many-body behaviour modifies the two-atom to molecule process that is so well characterised for slow rates of change of a parameter in the Hamiltonian to a many-body behaviour characterised by a power-law dependence on the sweep rate for the conversion process.

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