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Ultracold Bosons in a Tilted Multilevel Double-Well Potential

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The *N*-body problem in a tilted double well requires new features for macroscopic quantum superposition in ultracold atoms. In particular, one needs to go beyond the single-particle ground state in each well. We provide explicit criteria for when two energy levels are needed to describe the state space. For typical experimental parameters, two levels are indeed required for the creation of macroscopic superposition states. Furthermore, we show that a small tilt causes the collapse of such states. However, partial macroscopic superposition states reappear when the tilt can be compensated by atom-atom interactions.

Recently, Bose-Einstein condensates (BECs) in double-well potentials have been the subject of diverse and exciting research. For instance, such systems can be used to search for deviations from Newtonian gravity at small distances [1,2] and to store and retrieve optical information [3]. Interest in these systems is not limited to practical applications; BECs in double-well potentials also provide an ideal medium for the study of fundamental quantum many-body phenomena, such as macroscopic quantum tunneling [4–8] and macroscopic superposition (MS) states [9–12]. To describe these double-well systems, a Hubbard-like Hamiltonian has often been employed [13,14]. However, these studies not only assume that the trapping potential is symmetric, but effects of excited levels are completely neglected. Variational methods have indicated that excited levels play a significant role [15–17]. Moreover, a *multilevel* picture of a *tilted* double-well potential is *required* for the creation of a quantum computer from neutral atoms [18,19], atom-chip-based gravity sensors [1,2], and in the study of quantum transport phenomena [20–22]. Thus, the current experimental context of double-well potentials has created an urgent need for a new theoretical analysis of the many-body double-well problem.

In this Letter, we use a two-level Hamiltonian to investigate the stationary states of a BEC in a tilted, one-dimensional (1D), double-well potential. A schematic of our potential is shown in the inset of Fig. 1. In addition to interaction with the electromagnetic vacuum [9], thermal effects [11], and dissipation [12], we find that tilt also causes the collapse of MS states when the barrier is high, an effect we term *potential decoherence*. Unlike for other forms of decoherence, such states reappear when the tilt is compensated by atom-atom interactions. We call this a *tunneling resonance* because tilt suppresses tunneling between wells except when these states reappear [23,24]. Finally, we present novel, formal bounds for the use of a one-level approximation. This approximation is typically thought to hold when the interaction energy is much smaller than the energy level difference [17]. However,

we show that the effects of the excited energy level cannot be neglected even in this regime.

Past studies of the *N*-body double-well problem have focused on symmetric traps with one allowed energy level. Such systems map onto other physical problems, including a classical nonrigid pendulum [6] and the Lipkin-Meshkov-Glick model from nuclear physics [25]. Moreover, a double-well potential coupled to a heat bath can be used to study vibration modes in water molecules [26]. For the symmetric one-level model, tunneling dynamics [6–8,13] and the response to changes in experimental parameters such as barrier height have been analyzed [9,10,27] in various regimes. The behavior of the ground state energy in a *tilted* double-well has been studied in the one-level approximation [23]; however, applications such as quantum information processing [18,19] call for a two-level description. In our study of the double-well potential, we
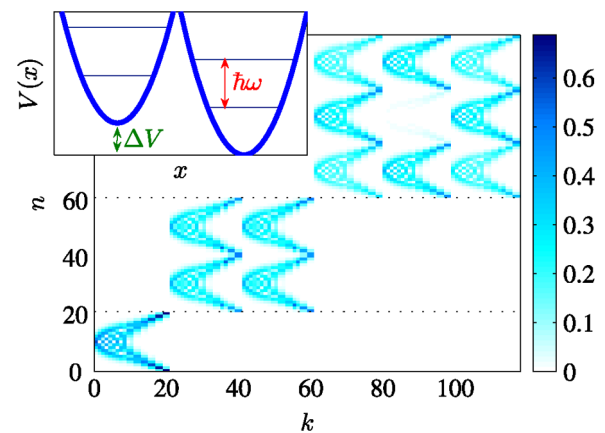

FIG. 1 (color online). *Energy eigenstates of a symmetric double well.* Shown are the probability amplitudes $|c_n^{(k)}|$ for a small range of Fock index n and energy eigenstate index k. Amplitude is indicated by hue. The total number of atoms is $N = 20$; above the dotted line at Fock index $n = 20$, one atom occupies the higher energy level; above the dotted line at $n = 60$, two atoms occupy the higher level, etc. Inset: schematic of the double-well potential.

relax two assumptions commonly made in previous studies of similar systems: the symmetric trap assumption and the one-level assumption. This leads to two new energy scales in our problem.

An approximate two-level Hamiltonian for N weakly interacting bosons in a tilted double-well potential is

$$\hat{H} = \hat{H}^0 + \hat{H}^1 + \hat{H}^{01}, \tag{1}$$

where

$$\hat{H}^\ell \equiv -J^\ell \sum_{j \neq j'} \hat{b}_j^{\ell\dagger} \hat{b}_{j'}^\ell + U^\ell \sum_j \hat{n}_j^\ell (\hat{n}_j^\ell - 1)$$
$$+ (\Delta V/2)(\hat{n}_L^\ell - \hat{n}_R^\ell) + E^\ell (\hat{n}_L^\ell + \hat{n}_R^\ell), \tag{2}$$

is the usual one-level Hamiltonian and

$$\hat{H}^{01} \equiv U^{01} \sum_{j, \ell \neq \ell'} (2\hat{n}_j^\ell \hat{n}_j^{\ell'} + \hat{b}_j^{\ell\dagger} \hat{b}_j^{\ell\dagger} \hat{b}_j^{\ell'} \hat{b}_j^{\ell'}), \tag{3}$$

couples the energy levels. Here, $[\hat{b}_j^\ell, \hat{b}_{j'}^{\ell'\dagger}] = \delta_{jj'}\delta_{\ell\ell'}$, $[\hat{b}_j^{\ell\dagger}, \hat{b}_{j'}^{\ell'\dagger}] = [\hat{b}_j^\ell, \hat{b}_{j'}^{\ell'}] = 0$, and $\hat{n}_j^\ell \equiv \hat{b}_j^{\ell\dagger} \hat{b}_j^\ell$. Equation (1) can be derived from first principles quantum field theory for weakly interacting bosons at zero temperature [28]. The superscripts $\ell, \ell' \in \{0, 1\}$ are the energy level indices, the subscripts $j, j' \in \{L, R\}$ are the well or site indices, J^ℓ are the tunneling energies, U^ℓ and U^{01} are the interaction energies, E^ℓ is the energy of the ℓth excited level, and ΔV is the tilt. Setting $E^0 = 0$, the energy difference between levels, or level spacing, is $E^1 \equiv \hbar\omega$. The extension of Eq. (1) to an infinite number of sites leads to the two-band Bose-Hubbard Hamiltonian.

The two-level Hamiltonian allows for on-site interactions, tunneling between wells, and hopping between levels. The tunneling terms J^ℓ allow single particles to tunnel between wells in the same level. Pairs of particles in the same well interact with interaction energy U^ℓ if they are in the same energy level and U^{01} if they are in different levels. Interactions can be either repulsive, $U^\ell > 0$, or attractive, $U^\ell < 0$. Furthermore, while single-atom transitions between energy levels are forbidden, *two* atoms can hop together between energy levels with amplitude U^{01}. Thus, the energy levels are coupled by the interlevel interaction energy U^{01}. Interactions between atoms in different wells are much smaller than U^0 and have been neglected in Eq. (1). The parameters J^ℓ, $\hbar\omega$, and U^ℓ are determined by overlap integrals of the localized single-particle wave functions. Left- and right-localized wave functions are constructed by superpositions of the appropriate symmetric and antisymmetric eigenfunctions of the single-particle Hamiltonian. While the interaction and tunneling energies are independent parameters, J^ℓ and $\hbar\omega$ are not. The tunneling and interaction energies satisfy $J^0 \ll J^1 \ll \hbar\omega$, $U^1 = (3/4)U^0$, and $U^{01} = (1/2)U^0$. In Figs. 1–3, we set $J^0/\hbar\omega = 4 \times 10^{-7}$ and $J^1/\hbar\omega = 3 \times 10^{-5}$. Finally, we note that the use of single-particle wave functions and only a few levels is appropriate to the regime $|NU^0| \lesssim 2\hbar\omega$. When $|NU^0| \gtrsim 2\hbar\omega$, our approximation is inaccurate, and alternative treatments become necessary [16,17,29].

An arbitrary state vector in Fock space is given by

$$|\Psi\rangle = \sum_{n=0}^{\Omega-1} c_n |n\rangle, \qquad |n\rangle \in \{|n_L^0, n_R^0\rangle \otimes |n_L^1, n_R^1\rangle\}, \tag{4}$$

where n_j^ℓ is the number of particles in the ℓth level of the jth well. We require the total number of particles in the double well, $N \equiv \sum_{j,\ell} n_j^\ell$, to be constant. The Fock index n increases with n_L^0, $n_L^0 + n_L^1$, and n_L^1. The dimension of the Hilbert space is $\Omega \equiv (N + 3)(N + 2)(N + 1)/6$; in the one-level approximation, this reduces to simply $N + 1$. The energy eigenstates and eigenvalues of the Hamiltonian (1) are given by $\hat{H}|\phi_k\rangle = \varepsilon_k |\phi_k\rangle$, for $0 \leq k \leq \Omega - 1$. The probability amplitudes are defined as $c_n^{(k)} \equiv \langle n|\phi_k\rangle$ for $0 \leq n \leq \Omega - 1$. Throughout our treatment, we consider the regime $|NU^0| \ll 2\hbar\omega$. Furthermore, we work in the high barrier limit $J^0 \ll |U^0|$, as it is instrumental to the creation of stationary MS states. For simplicity, we restrict our discussion to repulsive interactions, $U^0 > 0$ and positive tilt, $\Delta V > 0$. However, our results hold for $U^0 < 0$ and $\Delta V < 0$ as well.

Characteristic eigenstate amplitudes are shown in Fig. 1 for a symmetric trap. For a given n, the number of particles in the excited level is equal to the number of horizontal dashed lines below n. In the case of Fig. 1, mixing of levels is negligible. The lowest excited group of eigenstates, for instance, corresponds to full occupation of the lowest level. Likewise, the eigenvalues occur in $N + 1$ groups approximately separated by the level spacing $\hbar\omega$. As the number of particles, the interaction energy, or the tilt increases, the spacing between groups decreases, as in Figs. 2(a) and 2(b). In a symmetric trap, the first of many eigenvalue crossings occurs when the condition

$$U^0 \lesssim U_{\text{crit}}^0 \equiv 2\hbar\omega/(N^2 - 1), \tag{5}$$

is violated. When $U^0 \gtrsim U_{\text{crit}}^0$, MS states with nonzero occupation of the excited level emerge among the first $N + 1$ eigenstates, and a two-level approximation must be used. As the interactions increase, the lowest eigenstates include MS states with successively larger occupation of the excited level. Eventually, even the ground state will have significant contributions from the excited level. In a tilted potential, condition (5) becomes

$$\Delta V \lesssim \Delta V_{\text{crit}}$$
$$\equiv \begin{cases} \hbar\omega/N, & U^0 \leq U_{\text{max}}^0 \\ 2U^0[\sqrt{1 + 2(\hbar\omega/U^0)} - N], & U^0 > U_{\text{max}}^0 \end{cases}, \tag{6}$$

where we have defined $U_{\text{max}}^0 \equiv U_{\text{crit}}^0(N + 1)/(4N)$. These results can be obtained formally in the limit of small tunneling. In the opposite, noninteracting limit, we have developed a formal criterion involving the hopping as well [28]: $N < 1/2 + (\hbar\omega - J^1)/(2J^0)$.

While direct product states are not true eigenstates of the two-level Hamiltonian for $U^0 > 0$, the $N + 1$ lowest excited eigenstates have negligible contributions from the
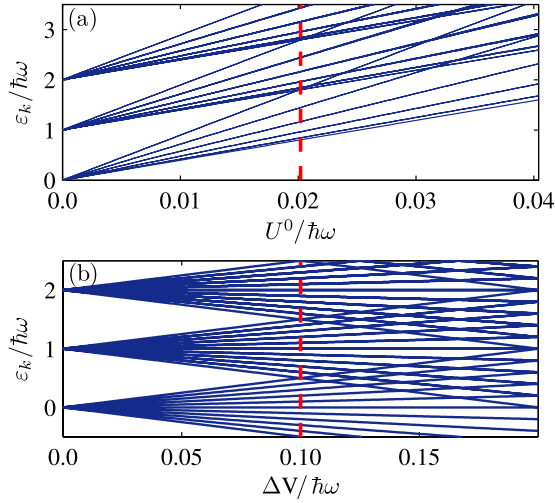
FIG. 2 (color online). *Breakdown of the one-level approxima-tion.* Energy eigenvalues versus (a) interaction energy with $\Delta V = 0$ and (b) tilt with $J^0/U^0 = 0.1$ for a ten-atom system. The thick dashed lines in panels (a) and (b) correspond to $U^0 = U^0_{crit}$ and $\Delta V = \Delta V_{crit}$, respectively. Eigenvalue crossings cause states with nonzero occupation of the excited energy level to emerge among the $N + 1$ lowest-lying eigenstates.

FIG. 3 (color online). *Potential decoherence and tunneling resonances.* Eigenstate probability amplitudes for a small range of Fock index n and eigenstate index k for $N = 10$, $J^0/U^0 = 0.1$, and (a) $\Delta V/U^0 = 0$, (b) $\Delta V/U^0 = 10^{-2}$, and (c) $\Delta V/U^0 = 6$. (b) A small tilt collapses the stationary macroscopic superposi-tion (MS) states. (d) Avoided crossings in the energy eigenvalues indicate a reappearance of partial MS states, as in (c).

excited level when conditions (5) and (6) are met. In a symmetric potential, these states are of the form

$$|\phi_\pm; \nu\rangle = |\Psi_\pm; \nu\rangle \otimes |0, 0\rangle, \qquad (7)$$

to $(N - 2\nu - 1)$th order in J^0/U^0 for $0 \leq \nu < N/2$. Here,

$$|\Psi_\pm; \nu\rangle \equiv (|\nu, N - \nu\rangle \pm |N - \nu, \nu\rangle)/\sqrt{2} \qquad (8)$$

represent *partial* MS states. To $(N - 2\nu)$th order in J^0/U^0, the energy difference $\Delta\varepsilon_\nu$ of antisymmetric $(-)$ and sym-metric $(+)$ pairs of states is

$$\Delta\varepsilon_\nu = \frac{4U^0[J^0/(2U^0)]^{N-2\nu}(N - \nu)!}{\nu![(N - 2\nu - 1)!]^2}, \qquad (9)$$

which is a very small number. In the presence of a high barrier, the eigenstates therefore occur in nearly degenerate pairs of entangled states [9,10] when the potential is sym-metric. Here, $\nu = 0$ represents the *extreme* MS state in which all atoms simultaneously occupy both wells. Characteristic probability amplitudes for the $N + 1$ lowest eigenstates are shown in Fig. 3(a).

Because the level splitting between antisymmetric and symmetric pairs is so small, small perturbations can mix these states [9] and produce a localized state of the form $|\nu, N - \nu\rangle \otimes |0, 0\rangle$. Indeed, MS states are highly sensitive to tilt ΔV, as illustrated in Fig. 3(b). The MS states of Eq. (7) are destroyed when

$$\Delta V \gtrsim 2\Delta\varepsilon_\nu/(N - 2\nu). \qquad (10)$$

Small imperfections in the external potential thus consti-tute a source of quantum decoherence. In addition to dis-sipation and measurement, potential decoherence therefore poses a further difficulty in the engineering of MS states in
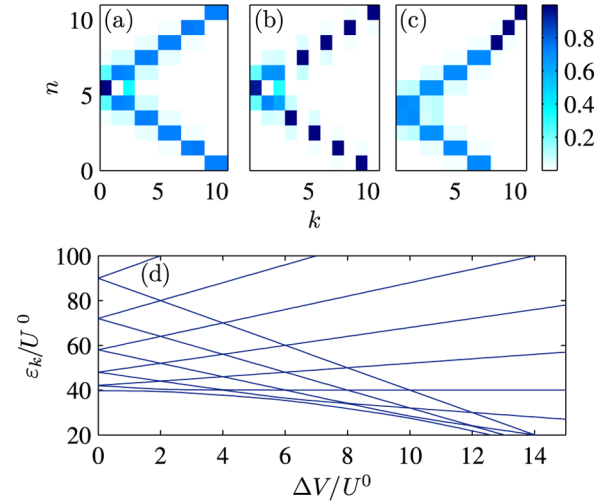
experiments. Because condition (10) is minimized when $\nu = 0$, extreme MS states are the most sensitive to imper-fections in the double well, making them an unlikely can-didate for experiments. Partial MS states, $\nu > 0$, on the other hand, are more robust with respect to potential deco-herence [30].

Despite their fragility, MS states reappear periodically for certain values of the tilt. Such resonances occur when

$$\Delta V = \Delta V_p \equiv 2pU^0, \qquad p \in \{1, 2, \dots, N - 1\}. \quad (11)$$

In this case, the potential difference can be exactly com-pensated by the interaction of p atoms in the lower well. To $(N - 2\nu - p - 1)$th order in J^0/U^0, the energy eigen-states are partial MS states of the form

$$|\phi_\pm; \nu, p\rangle = |\Psi_\pm; \nu, p\rangle \otimes |0, 0\rangle, \qquad (12)$$

$$|\Psi_\pm; \nu, p\rangle \equiv (|\nu, N - \nu\rangle \pm |N - \nu - p, \nu + p\rangle)/\sqrt{2}, \qquad (13)$$

for $0 \leq \nu < (N - p)/2$. The reappearance of MS states is shown in Fig. 3(c) for $\Delta V = \Delta V_3$, i.e., the third resonance. Because these states also occur in nearly degenerate pairs, the tunneling resonances are easily identified by avoided crossings in the energy eigenvalues, such as those dis-played in Fig. 3(d). At odd integer values of $\Delta V/U^0$, the eigenstates are maximally localized with the largest energy splitting between pairs of states. Near a resonance, the eigenstates become localized when

$$|\Delta V - \Delta V_p| \gtrsim 2\Delta\varepsilon^p_\nu/(N - 2\nu - p), \qquad (14)$$

where $\Delta\varepsilon^p_\nu \propto (J^0/U^0)^{N-2\nu-p}$ is the energy difference be-tween the states $|\phi_-; \nu, p\rangle$ and $|\phi_+; \nu, p\rangle$. For the special

case $\nu = 0$, we find

$$\Delta\varepsilon_0^p = \frac{4U^0[J^0/(2U^0)]^{N-p}(N-p)}{(N-p-1)!}\sqrt{\frac{N!}{p!(N-p)!}}, \quad (15)$$

to $(N-p)$th order in J^0/U^0. Tunneling resonances are vital in systems in which tilt is applied deliberately.

To demonstrate the robustness of the resonant MS states, we consider $N = 100$ ^{87}Rb atoms in a 1D analog of the double-well potential of Ref. [18]:

$$V(x) = -\upsilon_1\cos^2(2kx) - \upsilon_2\cos^4(kx - \pi/4 - \theta), \quad (16)$$

for $kx \in [-\pi/4, 3\pi/4]$, $\upsilon_2/\upsilon_1 < 2$, and $\theta \in [0, \pi/4]$. Here, $k = 2\pi/\lambda$ where $\lambda = 810$ nm. We set $\upsilon_1 = \upsilon_2/0.15 = 106E_r$ where $E_r/\hbar = 2\pi \times 3.5$ kHz is the recoil energy of the lattice [31]. The radial trapping frequency is $\omega_\perp = 2\pi \times 3.2$ kHz. For such a potential, $\hbar\omega/E_r = 36$, $NU^0/(2\hbar\omega) = 0.10$, and $J^0/U^0 = 0.10$. The critical interaction energy and tilt are $U^0_{\text{crit}}/U^0 = 0.10$ and $\Delta V_{\text{crit}}/E_r = 0.36$, respectively. In a symmetric trap, $\theta = 0$, the extreme MS states $|\phi_\pm; 0, 0\rangle$ will collapse for deviations in the tilt on the order of $10^{-287}E_r$. However, at the 98th resonance, i.e., when $\Delta V = \Delta V_{98} = 14E_r$, the few-atom MS state $|\phi_\pm; 0, 98\rangle$ can withstand deviations in the tilt up to $\pm 0.098E_r$. The 98th resonance corresponds to $\theta = 0.52 \pm 1.2\%$ [32]. Clearly, the many-body wave function protects partial MS states; a MS state of a few atoms *without* the presence of a many-body cushion is not experimentally realistic [24].

In conclusion, we have shown that not one, but three energy scales are required to describe macroscopic superposition states of ultracold atoms in a double well: hopping, tilt, and energy level spacing, all in ratio to interaction. These energy scales arise naturally within the context of quantum information processing with neutral atoms. After solving the appropriate Hamiltonian, we showed that tilt is a prevalent source of quantum decoherence which cannot be neglected in experiments. Moreover, we provided simple, formally derived criteria for when all three energy scales are required. Our treatment of the two-level double-well potential was restricted to 1D for simplicity. While all considerations made here also apply to 2D and 3D, there is one very important difference. In the latter case, angular momentum associated with the excited state in each well introduces another quantum number, as we analyze in detail elsewhere [28].

[1] B. V. Hall et al., Phys. Rev. Lett. **98**, 030402 (2007).
[2] T. Schumm et al., Nature Phys. **1**, 57 (2005).
[3] N. S. Ginsberg, S. R. Garner, and L. V. Hau, Nature (London) **445**, 623 (2007).
[4] Y. Shin et al., Phys. Rev. Lett. **95**, 170402 (2005).
[5] M. Albiez et al., Phys. Rev. Lett. **95**, 010402 (2005).
[6] A. Smerzi, S. Fantoni, S. Giovanazzi, and S. R. Shenoy, Phys. Rev. Lett. **79**, 4950 (1997).
[7] G. J. Milburn, J. Corney, E. M. Wright, and D. F. Walls, Phys. Rev. A **55**, 4318 (1997).
[8] I. Zapata, F. Sols, and A. J. Leggett, Phys. Rev. A **57**, R28 (1998).
[9] Y. P. Huang and M. G. Moore, Phys. Rev. A **73**, 023606 (2006).
[10] K. W. Mahmud, H. Perry, and W. Reinhardt, Phys. Rev. A **71**, 023615 (2005).
[11] L. Pitaevskii and S. Stringari, Phys. Rev. Lett. **87**, 180402 (2001).
[12] P. J. Y. Louis, P. M. R. Brydon, and C. M. Savage, Phys. Rev. A **64**, 053613 (2001).
[13] A. P. Tonel, J. Links, and A. Foerster, J. Phys. A **38**, 1235 (2005).
[14] R. W. Spekkens and J. E. Sipe, Phys. Rev. A **59**, 3868 (1999).
[15] C. Menotti et al., Phys. Rev. A **63**, 023601 (2001).
[16] O. Alon and A. Streltsov, and L. Cederbaum, Phys. Lett. A **362**, 453 (2007).
[17] D. Ananikian and T. Bergeman, Phys. Rev. A **73**, 013604 (2006).
[18] J. Sebby-Strabley, M. Anderlini, P. S. Jessen, and J. V. Porto, Phys. Rev. A **73**, 033605 (2006).
[19] T. Calarco et al., Phys. Rev. A **70**, 012306 (2004).
[20] Q. Niu, X.-G. Zhao, G. A. Georgakis, and M. G. Raizen, Phys. Rev. Lett. **76**, 4504 (1996).
[21] S. R. Wilkinson et al., Phys. Rev. Lett. **76**, 4512 (1996).
[22] A. Tomadin, R. Mannella, and S. Wimberger, Phys. Rev. Lett. **98**, 130402 (2007).
[23] A. P. Tonel, J. Links, and A. Foerster, J. Phys. A **38**, 6879 (2005).
[24] D. R. Dounas-Frazer and L. D. Carr, arXiv:quant-ph/0610166 (unpublished).
[25] J. Vidal, G. Palacios, and C. Aslangul, Phys. Rev. A **70**, 062304 (2004).
[26] S. Flach, V. Fleurov, and A. A. Ovchinnikov, Phys. Rev. B **63**, 094304 (2001).
[27] A. K. Tuchman, C. Orzel, A. Polkovnikov, and M. A. Kasevich, Phys. Rev. A **74**, 051601(R) (2006).
[28] D. R. Dounas-Frazer, Master's thesis, Colorado School of Mines, 2007.
[29] D. Masiello, S. B. McKagan, and W. P. Reinhardt, Phys. Rev. A **72**, 063624 (2005).
[30] These states are also more robust with respect to interactions with the electromagnetic vacuum [9].
[31] A more realistic barrier height $\upsilon_1 = 40E_r$ can be used to access the regime $J^0/U^0 \ll N$. While this regime still supports tunneling resonances, there are two important differences. First, there are less than $N-1$ resonances. Second, while Eqs. (11) and (14) still describe resonances, Eqs. (9) and (15) require higher orders of J/U.
[32] Although $U^0 > U^0_{\text{crit}}$ and $\Delta V_{98} > \Delta V_{\text{crit}}$, tunneling resonances are still described by Eqs. (11) and (14).