Breakdown of an Electric-Field Driven System: a Mapping to a Quantum Walk

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(Dated: April 1, 2022)

Quantum transport properties of electron systems driven by strong electric fields are studied by mapping the Landau-Zener transition dynamics to a quantum walk on a semi-infinite one-dimensional lattice with a reflecting boundary, where the sites correspond to energy levels and the boundary the ground state. Quantum interference induces a distribution localized around the ground state, and a delocalization transition occurs when the electric field is increased, which describes the dielectric breakdown in the original electron system.

PACS numbers: 05.40.Fb,05.60.Gg,72.10.Bg

Dynamics of quantum statistical systems driven by finite external fields has attracted much attention as a typical class of non-equilibrium phenomenon. One problem is the “dissipation” arising in electron systems driven out of their ground states by strong electric fields as studied by many authors [1, 2, 3, 4, 5, 6, 7]. In these references the electric field is expressed (via Faraday’s electro-magnetic induction) as a time-dependent Aharonov-Bohm(AB) flux, and this induces, for strong fields, interlevel Landau-Zener transitions. There, an issue is whether the bunch of energy levels around the zero level anti-crossings (as schematically shown in Fig.1(a)), which come from the disorder in disordered (one-body) systems, or from Umklapp processes in correlated systems. The system obeys the time-dependent Schrödinger’s equation starting from the ground state $|\Psi_0\rangle$ of $H(0)$, where its formal solution is $Te^{-i\int_0^t H(\phi(s))ds}|\Psi_0\rangle$. When the field is finite, non-adiabatic Landau-Zener tunneling processes occur at the level anti-crossings, which take place first from the ground state and then among higher excited states. Authors of [1, 3, 4] introduced a transfer matrix representation to mimic the evolution $Te^{-i\int_0^t H(\phi(s))ds}$, where a set of $2 \times 2$ unitary matrices represent the transitions among neighboring energy levels. Extensive studies on this model have found the existence of a dynamical localization[8], or an Anderson localization in energy space[9]. However, the effect of quantum interference, which should be the key to the Anderson localization, has been studied only numerically[1, 2, 3, 4].

Now we want to point out that the Landau-Zener transitions in multi-level systems presented above can be mapped to a quantum walk on a lattice. We shall show that the localization (in energy axis) of wave functions can be studied in terms of an exact solution for the transition amplitudes in the quantum walk. Quantum walk is a quantum counterpart of the random walk[9, 10, 11]). The quantum walk model for studying the problem. We start by noting that the driven quantum system and the quantum algorithmic model have in fact similarities: The former deals with quantum transitions among macroscopic number of qubits governed by quantum logic gates, for which powerful analytical techniques are being developed.

In the one-dimensional tight-binding model, the Hamiltonian is $H(\phi(t)) = -t \sum_{i,\sigma} \left[ e^{-i\frac{2\pi}{\hbar}\phi(t)} c^\dagger_{i+1,\sigma} c_{i,\sigma} + \text{h.c.} \right] + V$, where $c^\dagger_{i,\sigma}$ creates an electron at $i = 1, 2, \ldots L$ with spin $\sigma = \uparrow, \downarrow$, the AB-flux measured in units of the flux quantum $\phi(t) = FLt/h$ represents the electric field $F$, and $V$ the external potential or electron-electron interaction. Disordered mesoscopic systems[1, 2, 3, 4] have been treated with this Hamiltonian, which has been extended to a strongly correlated electron system by three of the present authors[2]. The adiabatic energy levels against $\phi$ have many level anti-crossings (as schematically shown in Fig.1(a)), which come from the disorder in disordered (one-body) systems, or from Umklapp processes in correlated systems. The system obeys the time-dependent Schrödinger’s equation starting from the ground state $|\Psi_0\rangle$ of $H(0)$, where its formal solution is $Te^{-i\int_0^t H(\phi(s))ds}|\Psi_0\rangle$. When the field is finite, non-adiabatic Landau-Zener tunneling processes occur at the level anti-crossings, which take place first from the ground state and then among higher excited states. Authors of [1, 3, 4] introduced a transfer matrix representation to mimic the evolution $Te^{-i\int_0^t H(\phi(s))ds}$, where a set of $2 \times 2$ unitary matrices represent the transitions among neighboring energy levels. Extensive studies on this model have found the existence of a dynamical localization[8], or an Anderson localization in energy space[9]. However, the effect of quantum interference, which should be the key to the Anderson localization, has been studied only numerically[1, 2, 3, 4].

Now we want to point out that the Landau-Zener transitions in multi-level systems presented above can be mapped to a quantum walk on a lattice. We shall show that the localization (in energy axis) of wave functions can be studied in terms of an exact solution for the transition amplitudes in the quantum walk. Quantum walk is a quantum counterpart of the random walk[4, 12, 13, 14]. The mapping we conceive here between the quantum walk and
the Landau-Zener dynamics is straightforward: A qubit on site \( n \geq 0 \) labeled by \( L, R \) corresponds to the states at the \( n \)-th anticrossing point, which moves down (\( L \); with a left-going current) or up (\( R \); right-going) in energy after the tunneling event (Fig. 1). One important point we note here is that the mapped quantum walk has a reflecting boundary, since we cannot walk below the ground state in energy. In previous quantum-walk studies \(^4\)\(^5\)\(^6\)\(^7\) an absorbing boundary was considered, for which the generating functions were obtained \(^4\). Here we first obtain the generating function for the quantum walk with a reflecting boundary. We have found the existence, and an analytic form for, the amplitude localized around the boundary (the ground state in the original problem). The solution exhibits an asymmetry between the \( L \) and \( R \) boundary (the ground state in the original problem). The solution exhibits an asymmetry between the \( L \) and \( R \) states, which represents a finite total momentum. When the electric field exceeds a critical value, a delocalization transition (on energy axis) is observed, which we identify as the backward scattering process. Here we simplify the problem by assuming that the matrices are the same \( U = \left( \begin{array}{cc} a & b \\ c & d \end{array} \right) \) except for the one at the boundary, \( \tilde{U} = \left( \begin{array}{cc} a & \tilde{b} \\ c & \tilde{d} \end{array} \right) \). As we shall see, an interesting structure arises in the overall shape of the distribution in the bounded quantum walk even within this simplification. The wave function evolves deterministically following a recursion formula,

\[
\Psi(n, \tau + 1) = P \Psi(n + 1, \tau) + Q \Psi(n - 1, \tau)
\]

(1)

for excited \((n \geq 2)\) states, while we put

\[
\Psi(1, \tau + 1) = P \Psi(2, \tau) + \tilde{Q} \Psi(0, \tau),
\]

\[
\Psi(0, \tau + 1) = P \Psi(1, \tau)
\]

(2)

between the ground and the first excited levels. Here we have decomposed \( U \) into \( P \equiv \left( \begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array} \right) \), \( Q \equiv \left( \begin{array}{cc} 0 & 0 \\ 0 & \tilde{1} \end{array} \right) \), and \( \tilde{Q} \equiv \left( \begin{array}{cc} 0 & 0 \\ a & b \end{array} \right) \). Equations (1, 2) define the mapping to a one-dimensional quantum walk on a semi-infinite space with a reflecting boundary at \( n = 0 \). We take the initial wave function \( |\Psi_0\rangle \) to be the ground state, i.e., \( \Psi(0, 0) = t(1, 0) \) and \( W(n, 0) = 0 \) for \( n \geq 1 \).

Generating function for the quantum walk — Now we state our main result for the quantum walk: We can obtain the generating function for the wave function in the reflecting boundary condition, where the generating function is defined as \( \Psi^{L,R}(0 \rightarrow n; z) = \sum_{\tau=0}^{\infty} \Psi_{L,R}(n, \tau) z^\tau \), with the summation taken over all the paths starting from 0 and ending at \( n \). The obtained expression is

\[
\Psi^L(0 \rightarrow n; z) = \left( \frac{d\lambda_+(z)}{a} \right)^n \frac{\tilde{c}d}{ac} \frac{\lambda_+(z) - az}{1 - \tilde{c}A'(0 \rightarrow 0; z)},
\]

\[
\Psi^R(0 \rightarrow n; z) = \left( \frac{d\lambda_+(z)}{a} \right)^n \frac{\tilde{c}d}{ac} \frac{\lambda_+(z) - 1 - \tilde{c}A'(0 \rightarrow 0; z)}{z^2}.
\]

(3)

Here \( \Delta \equiv \det U = ad - bc \), and \( A'(0 \rightarrow 0; z) = |d\lambda_+(z) - \Delta z|/c \) is the generating function for the quantum walk with an absorbing boundary, governed by Eqs. (1, 2) with \( \tilde{Q} = 0 \).

In order to obtain the generating function \( \tilde{Q} \), we first express the transition amplitudes \( \tilde{Z}_n(0 \rightarrow n; \tau) \) as a sum of the contributions from paths starting from the 0-th level (ground state) ending at the \( n \)-th level after \( \tau \) steps. For example, \( \tilde{Z}_n(0 \rightarrow 2; 4) = QPQ\tilde{Q} + PQ^2\tilde{Q} + Q\tilde{Q}P\tilde{Q} \). We also introduce \( \tilde{Z}_n(0 \rightarrow n; \tau) \) as the transition amplitude in the quantum walk with an absorbing boundary; e.g., \( \tilde{Z}_n(0 \rightarrow 2; 4) = QPQ\tilde{Q} + PQ^2\tilde{Q} \).

We obtain the transition amplitudes by employing a technique called the PQRS method \(^8\). Since the four matrices \( P, Q, R \equiv \left( \begin{array}{cc} c & 0 \\ 0 & c \end{array} \right) \) and \( S \equiv \left( \begin{array}{cc} 0 & b \\ b & 0 \end{array} \right) \), with \( \tilde{P}, \tilde{Q}, \tilde{R} \) defined similarly, span an orthonormal basis in \( M_2(\mathbb{C}) \) with an inner product \( \langle A|B \rangle = \text{Tr}(A^\dagger B) \), we can express the transition amplitude \( \tilde{Z}_n(0 \rightarrow n; \tau) \) as a linear combination,

\[
\tilde{Z}_n(0 \rightarrow n; \tau) = b^\tau(0 \rightarrow n; \tau)\tilde{Q} + \tilde{b}^\tau(0 \rightarrow n; \tau)\tilde{R}
\]

(4)

with the tilde basis, where \( \tilde{P} \) and \( \tilde{S} \) terms are absent. Thus, eq. (3) defines a set of complex numbers \( b^\tau(0 \rightarrow n; \tau) \) and \( \tilde{b}^\tau(0 \rightarrow n; \tau) \), and we denote \( \tilde{B}^\tau(0 \rightarrow n; z) = \sum_{\tau=0}^{\infty} b^\tau(0 \rightarrow n; \tau) z^\tau \) as their generating functions. The generating functions \( \tilde{A}^\tau(0 \rightarrow n; z) \) for the absorbing boundary problem are defined similarly from \( \tilde{Z}_n(0 \rightarrow n; \tau) \), \( \tilde{b}^\tau(0 \rightarrow n; \tau) \tilde{Q} + \tilde{a}^\tau(0 \rightarrow n; \tau) \tilde{R} \). We note that for \( n = 0 \) the \( \tilde{Q} \) terms vanish, i.e., \( \tilde{B}^\tau(0 \rightarrow 0; z) = A^\tau(0 \rightarrow 0; z) = 0 \). For a special case \( \tilde{U} = U \), we drop all the tilde marks \( \tilde{Z}_n(0 \rightarrow n; \tau), \tilde{B}^\tau(0 \rightarrow n; z), \tilde{b}^\tau(0 \rightarrow n; \tau) \)...

The PQRS method establishes a connection between the generating functions via multiplication rules \(^8\) for the \( PQRS \) matrices. From a recursion relation between
\[ \tilde{Z}^B(0 \to 0; \tau) \text{ and } \tilde{Z}^R(0 \to n-1; \tau-1), \] we obtain
\[ \tilde{B}^R(0 \to n; z) = \left[ 1 + i\tilde{B}^R (0 \to 0; z) \right] dzB^R (0 \to n-1; \tau); \]
\[ \tilde{B}^L (0 \to n; z) = \left[ 1 + i\tilde{B}^L (0 \to 0; z) \right] dzB^L (0 \to n-1; \tau). \]

With a repeated application of the no-tilde version of Eq. 3, we obtain
\[ B^R (0 \to n; z) = [d\lambda_+(z)/a]^n/d, \]
\[ B^L (0 \to n; z) = [d\lambda_+(z)/a]^n(\lambda_+(z) - az)/(acz)]. \]

Again using \( \tilde{\Delta} \) with a relation between \( \tilde{B}^L (0 \to 0; z) \) and \( \tilde{A}^R (0 \to 0; z) \), we arrive at eqs. 3 after a bit of algebra.

**Edge states in energy space** — One asset of the generating function is that we can show that there exist “edge states” in the bounded quantum walk. To actually show this let us take the Landau-Zener tunneling probability, \( p = \exp(-\pi F/F) \), where the Zener threshold electric field \( F \propto \Delta^2 \) depends on the size of the gap \( \Delta \).

We plug this in the transfer matrix,
\[ U = \left( \begin{array}{cc} -\sqrt{1-p}e^{i\beta} & \sqrt{1-p}\gamma \\ \sqrt{1-p}e^{i\gamma} & \sqrt{1-p}
\end{array} \right), \]
\[ \tilde{U} = \left( \begin{array}{cc} 0 & e^{i\gamma} \\ -e^{-i\gamma} & 0 \end{array} \right), \]
where the diagonal elements of \( \tilde{U} \) are set to zero to represent a complete reflection. The phases \( \beta, \gamma, \tilde{\gamma} \) consist of the dynamical phase and the geometric phase (nonadiabatic counterpart to Berry’s phase). In physical systems (such as the Hubbard model) these phases at the level anti-crossings are generally nonzero (and depend on the driving force \( F \)).

Expanding the generating function \( \Psi \) into a power series in \( z \) yields the time evolution of the wave function (Fig 2). We can see that \( \Psi \) (distribution on energy axis) breaks up, after a transient period, into two parts, \( \Psi (n, \tau) = \Psi_{\text{edge}} (n, \tau) + \Psi_{\text{bulk}} (n, \tau) \), where \( \Psi_{\text{edge}} \) is a component localized around the boundary (i.e., the ground state) while \( \Psi_{\text{bulk}} \) is a component traveling into the bulk (excited states) with a nearly constant velocity. Interestingly, the edge state only appears when the phase difference,
\[ \theta = \gamma - \tilde{\gamma}, \]
between the bulk and boundary transfer matrices is nonzero (as is the case with physical systems as mentioned).

What is the nature of the edge state? The two generating functions \( \Psi^{L,R}_{\text{edge}}(z) \) (eqs. 3) have a common, first-order pole in \( z^2 \) at \( z_{\text{pole}}^2 = \frac{1 - e^{-i\gamma(x)}}{1 - e^{-i\gamma(x)}} \). We can then obtain, with the Darboux’s method \( \psi \) of the asymptotic wave function, \( \Psi_{\text{edge}} (n, \tau) \to \exp(-i\epsilon \Delta t/2\hbar) \Phi_{\text{edge}} (n) \), which obeys Floquet’s theorem \( \Phi \) and the Floquet quasi-energy per period \( \epsilon/L = (F/2\pi) \arg z_{\text{pole}} \), a function of the electric field \( F \) since \( p = \exp(-\pi F/F) \) involves \( F \). We note that \( \epsilon \) can be expressed as \( \epsilon = -i\hbar \lim_{\tau \to \infty} \frac{1}{2} \ln \langle \Psi_0 (U(t)|\Psi_0 \rangle \), i.e., the asymptotic effective Hamiltonian of the system. An important observation here is that the elements of the Floquet state \( \Phi_{\text{edge}} (n) = \epsilon(\phi^L (n), \phi^R (n)) \) with \( \phi^L, \phi^R (n) = \sqrt{2} |z_{\text{pole}}^2| p/L \)

\[ \lim_{z^2 \to z_{\text{pole}}^2} \psi^{L,R} (0 \to n; z) |1 - z^2/z_{\text{pole}}^2\rangle, \]
form a geometric series,
\[ |\phi_L (n)\rangle^2 = r^n |\phi_L (0)\rangle^2, \]
\[ |\phi_R (n \geq 2)\rangle^2 = r^{n-1} |\phi_L (0)\rangle^2, \quad n = 0, 2, \ldots, \]
\[ r = p/(2p - 2c \theta \sqrt{1-p}), \]
with \( |\phi_L (0)\rangle^2 = (1 - r)^2 \). Thus \( \Phi \) (an edge state exponentially localized on energy axis) around the boundary \( n = 0 \), whose weight is \( \Phi^{\text{edge}} = \sum_n (|\phi_L (n)\rangle^2 + |\phi_R (n)\rangle^2) \), is \( 1 - r \). The size (on energy axis) of the edge state is \( \xi = 1/|\ln r| \), which behaves as \( \xi \propto F/F \) in the small \( F \) regime and diverges like \( |\ln F/F - \lim_{F \to \infty} \propto F/F \) in the vicinity of the threshold, \( \Phi_{\text{edge}} = \sqrt{\sin^2 \theta, F_{\text{edge}} = -\pi \sin \theta \Phi_{\text{edge}} = \sqrt{\sin^2 \theta, F_{\text{edge}} = \sqrt{\sin^2 \theta, F_{\text{edge}} = \sqrt{\sin^2 \theta, F_{\text{edge}} = \sqrt{\sin^2 \theta}}}. \]

When different paths meet, quantum interference induces localization of the wave function, and the edge state \( |\phi_{\text{edge}} (n)\rangle^2 \), occurring for \( \theta \neq 0 \), in the quantum walk problem represents an effect of such an interference. So the present result is an analytic version of the edge states observed numerically in the long-time limit (3).

The momentum and energy expectation values (summed over \( L \) and \( R \) states) for the edge state are
\[ J_{\text{edge}} = \sum_n [j_n^L |\phi_R (n)\rangle^2 + j_n^R |\phi_L (n)\rangle^2] / |\Phi_{\text{edge}}|, \]
\[ E_{\text{edge}} = \sum_n [E_n^L |\phi_R (n)\rangle^2 + E_n^R |\phi_L (n)\rangle^2] / |\Phi_{\text{edge}}|^2 \]

Here we normalize them by the total amplitude of the edge state \( |\Phi_{\text{edge}} (n)\rangle^2 \), which decreases as we increase.
B. Tregenna, et al., New J. Physics 5, 2002.

A similar model has been employed to analyze the critical situation to the edge-to-propagating transition in the quantum walk. At the breakdown point the energy expectation value diverges as \( E_{\text{edge}} \sim |F - F_c(\theta)|^{-2} \). The \( J_{\text{edge}} \), however, does not diverge but shows a smooth increase.

Discussions — The idea of mapping the non-equilibrium problem to a quantum walk may apply to wider range of systems having many energy gaps. Here we have concentrated on the “edge state” when there is randomness (i.e., \( \theta \neq 0 \)) only at the edge. Randomness in the transfer matrices in the excited state, ignored here, is expected to enhance the localization to bring \( |\Phi_{\text{edge}}|^2 \) closer to unity. Blatter et al. have in fact obtained the expectation value of the momentum in such a situation, where the result resembles \( J_{\text{edge}} \) obtained here. However, Blatter et al. did not obtain, in the range of electric field \( F \) they have studied, a delocalization transition. In fact, Cohen et al., in a random matrix model, found a disappearance of localized states in strong external fields. If such transitions also occur in electron systems, the quantum-walk picture may be used in understanding the transition. Indeed, some of the quantum-walk models now under study exhibit localization (e.g., [20]), and the present mapping may shed lights on the non-equilibrium properties of driven quantum systems.

It is a pleasure to acknowledge V. Kagalovsky, Y. Matsuo, S. Miyashita, N. Nagaosa, and Y. Tokura for fruitful discussions in the early stage of the present work. We also wish to thank M. Katori and T. Sasamoto who suggested a link between the Landau-Zener transition and quantum walks. One of us (TO) thanks the Yukawa Institute for Theoretical Physics at Kyoto University, where this work was initiated during the YITP-W-03-18 on “Stochastic models in statistical mechanics”. Part of this work was supported by a JSPS fellowship for Young Scientists.

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