Ground state wave function of the Schrödinger equation in a
time periodic potential.

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Abstract

Using a generalized transfer matrix method we exactly solve the Schrödinger equation in a
time periodic potential, with discretized Euclidean space-time. The ground state wave function
propagates in space and time with an oscillating soliton-like wave packet and the wave front is
wedge shaped. In a statistical mechanics framework our solution represents the partition sum
of a directed polymer subjected to a potential layer with alternating (attractive and repulsive)
pinning centers.

PACS numbers: 03.65.Ge; 68.35.Rh
Schrödinger equation plays a central role in modern physics. In the Euclidean space-time, the time is imaginary and the equation has interpretation in statistical mechanics. In contrast to the stationary case, i.e. equations in time independent potentials, where many exact solutions exist, for the general *time-dependent* situation exact results have been lacking so far.

In this work we present an exact solution, albeit in the Euclidean lattice space-time. We consider a periodic potential alternating between attractive and repulsive, placed at the space origin $x = 0$. The quantum analogue would be that of a particle in a forced potential with energy pumped in and out periodically. This problem has several links with important branches of modern theoretical physics. In the statistical mechanics framework our system, with a delta-like potential, is usually employed in the lattice models for wetting and depinning transitions of directed polymers [1], as well as it represents a simplified version (but nevertheless non trivial) of the KPZ equation for kinetic interface growth [2]. In a pure QM context the present problem has applications in: wave function collapse in mesoscopic systems, Mott-type hopping, transport in disordered systems, quantum electronics, time-dependent Zener tunneling (see [3] and references therein). Moreover it has been recently pointed out that the Schrödinger and diffusion equations are very deeply linked if represented on a lattice. In fact one can prove that, apart from the usual analytic continuation, they represent two aspects of the *same* probabilistic problem on a lattice manifold [4]. This maybe provides a new interesting interpretation of non-relativistic QM on a lattice.

The strategy of our approach is the following: we assume that at large times the wave function has the same periodicity of the potential. We also require that it is normalized for all times. For the symmetric case, i.e. when attractive and repulsive potentials have equal strength, the wave function is localized around the origin [5]. The normalized solution oscillates in the time direction and its amplitude is weaker and weaker when the spatial distance from the origin is larger and larger. Our wave function also shows that the wave front has a wedge shape as would be required by causality: the potential influence can only travel with finite velocity.
Let us start by considering the imaginary-time $d$-dimensional Schrödinger equation

$$\partial_t \Psi(x, t) = \left( \nabla^2 + \delta(x) \cos(\omega t) \right) \Psi(x, t),$$  

with the normalization $\int |\Psi(x, t)|^2 \, dx = 1$. Here we have considered the symmetric case: the time average of the potential is zero. However, our general solution also includes the nonsymmetrical situation. For sake of simplicity we will use the 1-$d$ notation for variables and operators even if we can work in a high dimensional space.

It can be shown that the above equation can be derived from a Hamiltonian which describes an elastic chain, or a directed polymer, in a periodic potential (alternatively attractive and repulsive). The Hamiltonian reads

$$H_L(\{h_k\}) = J \sum_{k=1}^L |h_{k+1} - h_k|^P - \sum_{k=1}^L u_k \delta_{h_k,0},$$

and, more specifically, it gives the energy of a polymer in a $(d + 1)$-dimensional space under the competing effect of the pure tension term proportional to $J$ and the potential layer at the origin. Here $h_k$ defines the position of the polymer at “time” $k$, while $u_k$ is set to $u > 0$ for even $k$ and $-v < 0$ for odd $k$. In the usual lattice version, one introduces RSOS conditions, that is the height difference $|h_{k+1} - h_k|$ can only take values 0 or 1 and overhangs are forbidden. Mathematically speaking, this is completely equivalent to assume $p = \infty$. The first term in (1) discourages large humps of the polymer (it corresponds to the laplacian in (1)), while the second term gives a positive (resp. negative) contribution to the total energy when the particle passes through the origin for odd (resp. even) times $k$. Hence it is the discretized (and non symmetric) form of the continuous sinusoidal potential in the original Schrödinger equation.

The equilibrium state of the polymer, whose energy is defined in (2) for a given configuration, is the result of the competition between two contrasting effects. At temperatures $T > 0$ we know from general arguments that large deviations from linearity increase the configurational entropy, but these jumps have also the effect of increasing the internal energy and a phase transition occurs at a given $T_c$ when the cost in energy is exactly balanced by the gain in entropy. This mechanism is completely specified by the free energy (per unit length) $f = F/L$. 

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From a geometrical point of view, below $T_c$, the polymer is localized in the sense that its mean variance from the origin remains finite in the thermodynamic limit $L \to \infty$. The opposite stands at $T > T_c$ in which the directed line behaves as a pure random walk in a $d$-dimensional space and performs thermal wandering. The QM counterpart of this phase transition is the binding/unbinding transition between eigenstates of the Hamiltonian defined in (1). After having clarified the mapping, our goal consists in the search of the partition function:

$$Z_L(x) = \sum_{\{h_k\}} e^{-\mathcal{H}_L(\{h_k\})/T},$$

(3)

which is the discretized Feynman path integral representation of the wave function associated to (1).

We then start by introducing the evolution equation for $Z_L(x)$ by means of a transfer matrix approach:

$$Z_{L+1}(x) = \left[ 1 + (a_{L+1} - 1)\delta_{x,0} \right] \times \left[ Z_L(x) + t \sum_{i=1}^{L} (Z_L(x + 1) + Z_L(x - 1)) \right].$$

(4)

The search of the ground state of eq.(1) is equivalent to the determination of the stationary solution of this recursion equation for $L \to \infty$. In the thermodynamic limit we know that only the largest eigenvalue $\varepsilon$ of the transfer matrix (4) gives a significant contribution to the free energy density, that is we have $f \simeq -\log\varepsilon$. We recall that, due to the particular form of the potential layer, we expect to find two distinct ground state wave functions in the bound regime, one for even ($\Psi_+$) and one for odd ($\Psi_-$) times.

The first step consists in the search of a self-consistent expression for the partition “wave” function. The full calculation has been already carried out in a general hypercubic lattice [8]: the result is that for any set of free parameters $\{d, u, v, J\}$ the normalized partition functions in the Fourier space $G_L^\pm(k) = Z_L^\pm(k)/(1 + 2dt)^L$ (with $t = \exp(-J/T)$) [7] satisfies the following implicit equation

$$G_{L+1}^\pm(k) = G_L^\pm(\xi(k)) + A \int_0^1 d^d q G_L^\pm(q)\xi(q),$$

(5)
where \( A = \exp(u/T) - 1 = A^+ \) for even times and \( A = \exp(-v/T) - 1 = A^- \) for odd times.

Moreover we have introduced the quantity \( \xi(k) = [1 + 2t \sum_{i=1}^{d} \cos(\pi k_i)]/(1 + 2dt) \). To take into account the periodicity of the potential layer we apply transformation (5) twice, so that we can relate \( G_{2L+2}^+ \) to \( G_{2L}^+ \) and \( G_{2L+1}^- \) to \( G_{2L-1}^- \). By using the ansatz, valid at large \( L \), \( G_L^+ (k) = \varepsilon^2 G_{L-2}^+(k) \) we finally get

\[
G^+ (k) = \frac{A^+}{\varepsilon^2 - \xi^2} K_2^+ + \frac{A^+ A^-}{(1 + 2dt)(\varepsilon^2 - \xi^2)} K_1^+ + \frac{A^- \xi}{\varepsilon^2 - \xi^2} K_1^+.
\]  

(6)

where we have introduced the two constants

\[
K_n^+ = \int_0^1 d^d q \xi^n(q) G_+ (q), \quad n = 1, 2.
\]  

(7)

We simply find, by symmetry, that \( G^- (k) \) can be derived from \( G^+ (k) \) by interchange between \( A^+ \) and \( A^- \). A phase transition occurs when the maximum eigenvalue converges towards \( 1^+ \), and it can be studied by means of the mass gap \( \mu \) defined as the inverse of the transversal correlation length, i.e. \( \Psi(x) \simeq \exp(-\mu x) \). One can prove that \( \varepsilon \simeq 1 + \mu^2 \) near the transition point \( 1^+ \). The r.h.s. of eq.(6) implicitly depends on \( G^\pm (k) \), the full knowledge of the wave functions would therefore require 4 independent equations for the constants \( K_{1,2}^\pm \). The first couple of equations can be simply derived from (6) by multiplying both sides for \( \xi(k) \) and integrating over the \( k \)-momentum. At the end we obtain the following identity

\[
K_1^+ \left( A^+ \mathcal{I}_2 + \frac{A^+ A^+}{1 + 2dt} \mathcal{I}_1 - 1 \right) + K_2^+ A^+ \mathcal{I}_1 = 0.
\]  

(8)

where

\[
\mathcal{I}_1 = \frac{1 + 2dt}{4t} \left( f_1(0) - g_1(0) \right),
\]

\[
\mathcal{I}_2 = \frac{1 + 2dt}{4t} \left( f_1(0) + g_1(0) \right) - 1,
\]  

(9)

and

\[
f_\varepsilon(x) = \int_0^{\infty} du e^{-\varepsilon u} I_{|x|}(u)^d,
\]

\[
g_\varepsilon(x) = \int_0^{\infty} du e^{-\varepsilon u} I_{|x|}(-u)^d.
\]  

(10)
In the above we have introduced the two quantities $\varepsilon_1 = \frac{\varepsilon(1+2dt)-1}{2t}$, $\varepsilon_2 = \frac{\varepsilon(1+2dt)+1}{2t}$ and we have used an integral representation of the modified Bessel function of integer order $I_n(u) = \int_0^1 \exp\{u \cos y\} \cos ny \, dy$. It is simple to convince oneself that any other attempt to find close equations for these constants from (6) would lead to relations which are not linearly independent respect to (8).

For the meanwhile we neglect the search of the second couple of equations and we concentrate on equation (6), which must be antitransformed in order to get the real space form of our solution. In performing the calculation we encounter non-trivial integrals of the form:

$$J_n(x) = \int_0^1 d^d k \prod_{i=1}^d \cos(\pi k_i x_i) \frac{\xi(k)^n}{\xi_2 - \xi_2(k)}, \quad n = 0, 1. \quad (11)$$

Without entering into mathematical details, we simply note that, by means of an appropriate Feynman integral representation, we can simplify them and after some more algebra we finally obtain that

$$J_0(x) = \frac{1+2dt}{4\varepsilon t} [f_\varepsilon(x) + g_\varepsilon(x)],$$

$$J_1(x) = \frac{1+2dt}{4t} [f_\varepsilon(x) - g_\varepsilon(x)]. \quad (12)$$

The symmetry of the system tells us that any function of $x$ must be invariant under axis reflection; this is why in the above integrals only the absolute value of $x$ appears. Note that after this manipulation, the dependence of our wave function on the spatial variable $x$ comes only from the order of the Bessel function involved in the integrals. Moreover, by using the property that $I_{|x|}(u)$ is an even (odd) function of the argument for even (odd) values of $|x|$ it is clear that our ground state solution has a particular oscillation as a function of $|x|$. As we will discuss below, this is nothing but a direct consequence of the alternating potential we have put at the origin. We also note that $f_\varepsilon(x)$ is a well known integral in the statistical mechanics context [8]: if one takes $\varepsilon = 1$ (or $\varepsilon = d$), it is associated to the total probability that a random walker, started from the origin, could finally reach a point $x$ in a $d$-dimensional cubic lattice. The divergence of $f_1(x)$ for $d < 3$ has also important consequences in the polymer depinning framework [3].
To summarize, our non-normalized wave function reads

$$\Psi_\pm(x) = \left( A^\pm K_2^\pm + \frac{A^\pm A^\mp}{1 + 2 d t} K_1^\pm \right) J_0(x) + A^\mp K_1^\pm J_1(x). \tag{13}$$

The above formula gives the qualitative behavior of our solution, but to get the full normalized wave function we also need a closed form for $K^\pm_{1,2}$. As we know that $\varepsilon > 1$ for a non zero mass gap, we can restrict to the localized phase and impose the correct normalization of the wave function. Therefore we ask that $\sum_x \Psi_\pm(x)^2 = 1$ in the real space, or equivalently, $\int_0^1 d^d k \, G_\pm(k)^2 = 2$ in the momentum space. This condition would give us the second couple of equations we needed to find $K^\pm_{1,2}$. Unfortunately the integrals resulting from (6) after this manipulation are much harder to handle with. In fact we find that the normalization condition reads

$$F_2(K_{1,2}^\pm, A^\mp) M_2 + F_1(K_{1,2}^\pm, A^\pm, A^\mp, d, t) M_1 + F_0(K_{1,2}^\pm, A^\pm, A^\mp, d, t) M_0 = 2, \tag{14}$$

where $F_0, F_1, F_2$ are some algebraic functions of their arguments and

$$M_n = \int_0^1 d^d k \, \frac{\xi^n(k)}{[\varepsilon^2 - \xi^2(k)]^2}, \quad n = 0, 1, 2. \tag{15}$$

We believe that no simple way can be found to simplify these high-dimensional integrals, and then at this point we are forced to restrict ourselves to the 1-$d$ case. In a pure statistical mechanics framework one could, in principle, ask $\Psi_\pm(x)$ to be sommable and not square-sommable. In this case we can perform all integrations and get the complete solution in all dimensions. Nevertheless, in the spirit of QM, in the present study we prefer to use the usual normalization of the square of $\Psi_\pm(x)$. At $d=1$ all previous integrals can be exactly solved and we find that

$$f_\varepsilon(x) = \frac{1}{\sqrt{\varepsilon_1^2 - 1} \left( \varepsilon_1 + \sqrt{\varepsilon_1^2 - 1} \right)^{|x|}},$$

$$g_\varepsilon(x) = \frac{(-1)^{|x|}}{\sqrt{\varepsilon_2^2 - 1} \left( \varepsilon_2 + \sqrt{\varepsilon_2^2 - 1} \right)^{|x|}}. \tag{16}$$
From these formulas we get immediately the result that the mass gap in the localized phase is given by \( \mu = \log(\varepsilon_1 + \sqrt{\varepsilon_1^2 - 1}) \) and then it vanishes, near the transition as \( \sqrt{\varepsilon - 1} \). This is, \textit{a posteriori}, the proof that the limit \( \varepsilon \to 1^+ \) gives the transition point, as previously stated.

By using (8) and (14) we can finally solve for \( K_{1,2}^\pm \):

\[
K_1^\pm = \sqrt{2I_1} \left\{ \left[ 1 - 2A^\mp I_2 + (A^\mp)^2 I_2^2 \right] M_0 + \left[ 2A^\mp I_1 - 2(A^\mp)^2 I_1 I_2 \right] M_1 + (A^\mp)^2 I_1 I_2^2 \right\}^{-1/2},
\]

\[
K_2^\pm = \left( \frac{1}{A^\mp I_1} - \frac{A^\mp I_2}{A^\mp I_1} - \frac{A^\mp}{1 + 2dt} \right) K_1^\pm. \tag{17}
\]

We now have the complete solution of our problem, since the ground state (bound) wave function is given by (13) with the coefficients defined in (17). In particular we find that, at \( d=1 \),

\[
M_2 = \frac{1}{4\varepsilon^3} (h_1 + h_2 + \varepsilon(l_1 + l_2)), \quad M_1 = \frac{1}{4\varepsilon} (l_1 - l_2), \quad M_0 = \frac{1}{4\varepsilon} (\varepsilon(l_1 + l_2) - h_1 - h_2), \tag{18}
\]

with

\[
h_{1,2} = \frac{1 + 2t}{2t} (\varepsilon_{1,2}^2 - 1)^{-1/2}, \quad l_{1,2} = (1 + 2t)^2 \frac{4t^2}{4t^2} \varepsilon_{1,2} (\varepsilon_{1,2}^2 - 1)^{-3/2}. \tag{19}
\]

After rearrangement of all the quantities we can now have a look of our result. The 1-d wave functions \( \Psi_+(x) \) and \( \Psi_-(x) \) are plotted in Fig.1 for a given set of parameters \( \{u, v, t\} \) in the localized phase. In order to check out the validity of our solution, we have performed some numerical simulations, and for any set of parameters we have found perfect agreement with the above analytical solution.

The information of the alternating potential at the origin propagates in the transversal direction with finite velocity, in a soliton-like fashion. This means that if we look at the shape of our solution in the space-time manifold we expect to find that the oscillations due to the alternating perturbation of the potential decrease by increasing the distance \( |x| \) from the origin and the wave front has the shape of a wedge (see Fig.2).
Performing the limit $\varepsilon \to 1^+$ we attain an unbound state: the peaks at the origin disappear and the two wave functions merge one over the other at diverging transversal correlation length (i.e. at vanishing $\mu = 1/\xi_\perp$). If one is interested at the behavior of the “gap” $\Delta_0 = \Psi_+(0) - \Psi_-(0)$ near the transition to an unbound state, then all information comes from the exponent $\alpha$, defined as $\Delta_0 \simeq (\varepsilon - 1)^\alpha$ for $\varepsilon \to 1^+$. From (13) and (17) we simply find that for $(\varepsilon - 1) \ll 1$ the gap reads $\Delta_0 \simeq \sqrt{(1+2t)/4(A^+K_1^- - A^-K_1^+)}$ and then two situations are possible: (i) we can converge to the critical point for generic $A^+ \neq A^-$ or (ii) we can attain a delocalized phase for $A^+ = A^-$. More precisely, in the second hypothesis, we approach the unbound state on the manifold $u = v$ and $u \to 0$ linearly with $\varepsilon - 1$. This difference is not trivial but rather reflects a physical property of our system: at $d = 1$ it has been proved that in the two above cases the phase transition is of 2nd. and 4th. order, respectively [5]. By taking the dominant contributions of the integrals defined in (9), (12) and (18) for $\varepsilon \to 1^+$ in the formulas (17) for $K_1^\pm$, after some calculations we find that $K_1^\pm \simeq (\varepsilon - 1)^{1/4}$. This result is the same in both cases described above, since the limit $u = v \to 0$ does not modify the leading order contribution in (17). Then we finally obtain that, depending on the way we approach the critical state, $\alpha = 1/4$ (i) or $\alpha = 5/4$ (ii) (recall that $A^\pm$ linearly converge to 0 for $\varepsilon \to 1^+$ in the last case). We finally remark that our solution, in a pure statistical mechanics context, has a certain relevance because it is the partition function associated to Hamiltonian (2), which describes, as above explained, the energy of a directed polymer in a periodic potential, a problem with several applications in statistical physics [2],[6].

In conclusion we have solved an imaginary time Schrödinger equation with a non-trivial time dependent potential on a lattice. The critical behavior separating localized and delocalized phases has interesting properties characterized by non trivial scaling exponents. We expect that the counterpart in continuum would have qualitatively same behavior, which may have in turn wider implications in the non-equilibrium quantum physics.
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Figure captions

Fig. 1
The wave functions $\Psi(x) = \Psi_+(x)$ and $\Phi(x) = \Psi_-(x)$ versus $x$ for the 1-d case in the bound state. The curves are obtained by smooth interpolation among the points given by the analytical solution on the lattice. Numerical simulations fit exactly the above curves for any set $\{u, v, J\}$ of free parameters.

Fig. 2
The full space-time shape of our wave function $\Psi(x, t)$. As explained in the text, the wave front is wedge-shaped. The two functions $\Psi_+$ (resp. $\Psi_-$) are easily found by intersecting the surface with a $t = \text{const.}$ plane for times $t$ such that $\Psi(x = 0, t)$ reaches a peak (resp. a valley).