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Stroboscopic wavepacket description of non-equilibrium many-electron problems

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Abstract

We introduce the construction of a orthogonal wavepacket basis set, using the concept of stroboscopic time propagation, tailored to the efficient description of non-equilibrium extended electronic systems. Thanks to three desirable properties of this basis, significant insight is provided into non-equilibrium processes (both time-dependent and steady-state), and reliable physical estimates of various many-electron quantities such as density, current and spin polarization can be obtained. The use of this novel tool is demonstrated for time-dependent switching-on of the bias in quantum transport, and new results are obtained for current-induced spin accumulation at the edge of a 2D doped semiconductor caused by edge-induced spin-orbit interaction.

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Wavepackets (WP) are a very useful concept when analyzing quantum mechanical scattering processes, since they combine local and wave-like aspects on an equal footing. Some of their more recent applications range from studies of the intrinsic spin Hall effect in semiconductors[1,2], spin-flip dynamics[3], thermal averaging and its influence on interference patterns[4] or transport of an electron through Luttinger liquid[5]. However, the use of traditional WPs in degenerate fermionic systems raises difficulties since the exclusion principle restricts the available eigenstates that are superposed within a single WP. Stevens[6] proposed wavepackets consisting of cut-off plane waves which facilitated inclusion of the exclusion principle and have been used for various problems in electronic transport[7]; however they do not directly relate to typical many-electron ensembles such as the electronic ground state or moderate perturbations from it at zero temperature.

If we forego the time-dependent feature of WPs, the latter problem is conveniently resolved with the introduction of Wannier functions[8,9]: by occupying a finite number of them, we locally recover the exact eigenstates of a system of non-interacting electrons.

In this work we combine the advantages of Wannier functions for extended systems with the time-dependent description of WP propagation. This is achieved by generalizing the orthogonal WPs introduced by Martin and Landauer[10] for ideal 1D leads. Our wave-packet basis set (WPB) has following three properties: (1) each basis function (WP) is localized in space, (2) occupying a subset of the WPB we recover the exact non-interacting many-electron ground state of a reference Hamiltonian, (3) the WPB is generated by time propagation through successive time-steps, τ, of *an initial set* of WPs, according to a reference Hamiltonian.

From the above properties it follows that we can view the whole basis set as a *stroboscopic pictures* of a continuous time-evolution of a suitably chosen family of *initial* WPs (Fig. 1). Since all WPs are orthonormal, each copy can be occupied by precisely one electron and in time τ each electron will move into its neighboring' WP. Similarly, if a single electron is in a superposition of several WPs, in time τ it will be in the *same* superposition but of the WPs obtained from the former by a single shift of the basis functions. This picture is valid as long as the reference Hamiltonian is time-independent in the region where the concerned WPs are localized. We will refer to this region as the *bulk* and to the rest, typically a much smaller region than the bulk, as the *scatterer*. Similarly, the bulk (scattering) WPs are those WPs that are generated with the bulk (bulk+scatterer) Hamiltonian.

To obtain the time-dependent dynamics in the scatterer one needs to perform a full time-dependent simulation of the bulk WPs entering the scatterer. However, the scattering WPs will

return into the bulk after some time, and there those WPs can once again be expanded into the bulk WPB and propagated as moves of length τ between the bulk WPs, i.e. analytically. Hence, the WPB offers a very simple interpretation of the processes as well as a framework to perform numerical time-dependent simulations.

The consistency of the conditions (1) and (3) demands that the reference Hamiltonian posses translational symmetry in the direction of propagation. Its eigenstates in the Bloch form will be sufficient to create a basis such that each WP from the initial set will be spatially localized and their time-propagated WPs will slowly disperse with increasing time. This property can be satisfied only if the reference Hamiltonian is just that of the bulk. We may also construct the WPB for the combined system where the reference Hamiltonian is that of bulk+scatterer, but it can be easily seen to lead to very non-local (scattering) WPs, as demonstrated in Fig. 1. However, the scattering-WPs' basis can be easily expanded into the bulk WPB, a fact of which we will make use later.

Definition of the WPB and its formal properties. To define the basis set let us take an extended system specified by the reference Hamiltonian $\hat{H}$ with a continuous spectrum of eigenen-

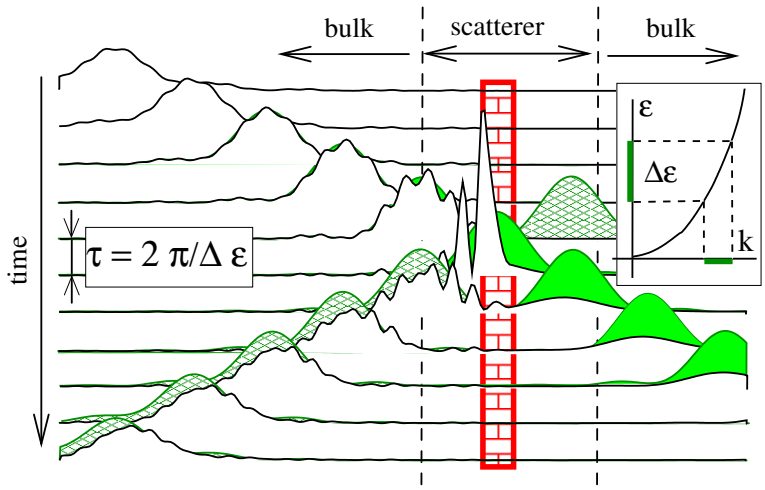

FIG. 1: Two examples of an orthogonal stroboscopic wavepacket basis (shown are the squared amplitudes of individual WPs). The white (scattering) WPs are obtained by propagation of the initial WP by a constant time-step τ dependent on the width of the invovled energy band (inset). Due to the scatterer the WPs become strongly delocalized (split). The alternative solid-green and green-meshed (bulk) WPs (right- and left-going respectively) generate a WPB that is localized; the former can be easily expanded into the latter.

ergies $\varepsilon \in (\varepsilon_0, \infty)$.

$$\hat{H}\,|\varepsilon,\alpha\rangle = \varepsilon\,|\varepsilon,\alpha\rangle\,.$$

To each eigen energy we will generally have a set of degenerate single-particle eigenstates[26] $|\varepsilon,\alpha\rangle\,, \quad \alpha = 1,2,...,N_\varepsilon$, forming all together a complete orthogonal whose normalization we choose such that

$$\langle \varepsilon',\alpha'|\varepsilon,\alpha\rangle = \delta(\varepsilon-\varepsilon')\delta_{\alpha,\alpha'}. \tag{1}$$

From the above set we can generate an orthogonal and complete wave-packet basis set (WPB) by first choosing the *initial set* of wave-packets

$$|n,0,\alpha\rangle = \frac{1}{\sqrt{\Delta\varepsilon_n}}\int_{\varepsilon_n^\alpha}^{\varepsilon_{n+1}^\alpha} d\varepsilon' U_{\alpha,\alpha'}(\varepsilon')\,|\varepsilon',\alpha'\rangle\,, \quad n = 0,1,2,... \tag{2}$$

for an arbitrarily chosen division of the spectrum into *energy bands* $\left\{(\varepsilon_n^\alpha, \varepsilon_{n+1}^\alpha)\right\}_{n=0}^{\infty}, \quad \alpha = 1,2,\ldots,N_\alpha$ with bandwidths $\Delta\varepsilon_n^\alpha = \varepsilon_{n+1}^\alpha - \varepsilon_n^\alpha$. The division into energy bands for each α must cover the full spectrum of $\hat{H}$ but otherwise can be chosen so as to achieve good localization and at the same time to suit the physical situation as discussed later. $U_{\alpha\alpha'}(\varepsilon)$ is a unitary, energy-dependent matrix that may be further specified to lead to maximally localized initial sets of WPs, in analogy with Wannier functions[9], or to adopt the bulk WPB to the scattering process in the scatterer. In our present applications we will use $U_{\alpha,\alpha'}(\varepsilon) = \delta_{\alpha,\alpha'}$ which is satisfactory and convenient for our present purposes. All the functions $\{|n,0,\alpha\rangle\}_n$ are orthogonal by definition, since they are linear combinations of eigenstates from disjunct energy bands.

The construction of the WPB is completed by forward and backward time propagation of the initial set

$$|n,m,\alpha\rangle = e^{-i\hat{H}m\tau_n}\,|n,0,\alpha\rangle\,, \quad m = \pm1,\pm2,\ldots \tag{3}$$

by regular, band-dependent time steps $\tau_n^\alpha = 2\pi/\Delta\varepsilon_n^\alpha$. It is easy to verify that this choice of time step *guarantees orthonormality of consecutive wave-packets within each band*

$$\langle n,m,\alpha|n,m',\alpha\rangle = \delta_{m,m'}. \tag{4}$$

Due to the orthogonality of the WPs we can uniquely expand any eigenstate of the reference Hamiltonian into the WPB with expansion coefficients (for $\varepsilon \in (\varepsilon_n, \varepsilon_n + \Delta\varepsilon_n)$)

$$\langle \varepsilon,\alpha|n,m,\alpha\rangle = \frac{1}{\sqrt{\Delta\varepsilon_n}} e^{-i\varepsilon m\tau_n}. \tag{5}$$

Conversely, combining Eqs.2, 3 and 5 one obtains that

$$\sum_m |n,m,\alpha\rangle \langle n,m,\alpha|\varepsilon,\alpha\rangle = |\varepsilon,\alpha\rangle\,, \tag{6}$$

from which follows that the WPB is also *complete* since the original set of eigenstates is a complete one.

It has been already pointed out that the division into bands can be exploited to optimize the basis set to the particular physical problem. A typical choice of the energy bands is to take $\varepsilon_n^\alpha = E_F$ for a cetrain n and all α, where E_F is the Fermi energy of the system. This way the ground-state is described by occupying all of the WPs in the bands below E_F. This means that we need to consider only few WP or electrons even though we are describing the *local* ground state properties of the infinite many-electron system exactly. Similarly, we can model non-equilibrium situation by imposing different effective Fermi energies for WPs with different values of α.

We will now demonstrate the use of the WPB on several examples from two rapidly developing areas of condensed matter physics - time-dependent and/or *ab initio* simulations in quantum transport, and spin accumulation due to spin-orbit coupling in 2D systems.

Time-dependent quantum transport. Understanding the quantum transport of charge through nanojunctions made of individual atoms or molecules will be essential for progress in nanoelectronics. Due to the short spatial scale and short times involved it is clear that transient phenomena play an important role in understanding the functionality of nanodevices. At the same time, it has been recognized that the correct treatment of interactions demandes a time-dependent formulation of the density- or current-density functional theory[11]. While several exact methods have been put forward[12,13,14,15], due to their inherent complexity, they give restricted insight into the processes involved. Here we show that the WPB can provide this insight in an elegant fashion, as well as quantitative estimates for quantities of interest such as transient time, oscillations or steady-state current.

As an example let us consider the simplest case possible - a 1D gas in which at time $t = 0$ a finite potential difference is applied (Fig. 2). This system was studied previously within the non-partitioning approach[13]. Anticipating the application of the bias ΔV, we split the occupied part of the spectrum of a Hamiltonian for free electrons into occupied bands 0 to ΔV, ΔV to $E_F - \Delta V$ and $E_F - \Delta V$ to E_F, and two unoccupied bands E_F to $E_F + \Delta V$ and $E_F + \Delta V$ to ∞. The continuum eigenstates fulfilling Eq. 1 are energy-normalized plane-waves $\langle x|\varepsilon,\alpha\rangle = e^{i\alpha kx}/\sqrt{2\pi k}, \quad k = \sqrt{2\varepsilon}$, and $\alpha = \pm$ for right- and left- going states respectively. (The resulting WPs are then identical to

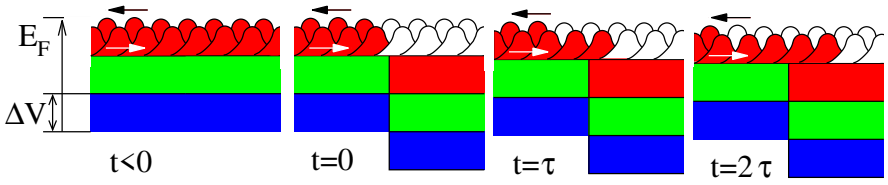

FIG. 2: Abrupt switching on of the bias in a simple 1D model of quantum transport of electrons. The three bands cover the occupied part of the spectrum. In response to the bias ΔV, the right-going WPs for $x > 0$ (the previously unoccupied band) start to fill the WPs from the left and the occupied left-going WPs for $x < 0$ become empty. The finite extent of each WP causes oscillations, with period τ, of the resulting current measured at any fixed x.

those employed by Martin and Landauer in the analysis of quantum noise[10].)

Switching on the bias ΔV at $x = 0$ and $t = 0$ will energetically align WPs from the highest occupied band and localized in $x < 0$ with the WPs from the lowest unoccpied band and localized in $x > 0$. A transient phenomenon for $t < t_{E_F} \sim 2\pi/E_F < \tau = 2\pi/\Delta V$, which can be analyzed only by actually performing a time-dependent simulation, will be related to dynamics of those occupied WPs that had for $t < 0$ nonzero amplitude for both $x < 0$ and $x > 0$. Apart from that the whole many-electron dynamics consists of consecutive filling of the empty right-going WPs for $x > 0$ and depleting the left-going WPs for $x < 0$. From this it follows that the current at fixed x_0, e.g. $x_0 = 0+$ will grow to its steady value $I = 2e/\tau = \Delta V/\pi$ (factor 2 for spin degeneracy of the WPs) in time t_{E_F}, accompanied by oscillations with period $T \sim \tau$ as the first WPs for $x > 0$ start to get occupied. The latter will decay as the tails of all WPs extending to x_0 get occupied. This behavior has also been obtained by with exact calculations based on non-equilibrium Greens functions within a wide band model[13].

The analysis of a system with a tunneling barrier at $x = 0$ (of transmission $t(\varepsilon)$) can be accomplished in a similar way. This time, it will not be a single whole WP for $x > 0$ being filled, but only a fraction of it, according to the expansion of the scattering WP into the bulk WPs (see Fig. 1). Therefore, the steady current $I = 2|\langle t(\varepsilon)\rangle|^2/\tau = (T/\pi)\Delta V$, where $\langle\ \rangle$ means average over the energies in the relevant band, and this steady value will be accompanied by oscillations decaying in amplitude. Furthermore, the phase shift of the scattering WPs carries information about the tunneling interaction time and density depletion/increase around the barrier. The use of the WPs' phase shift is discussed further in the application to spin accumulation below.

This result is valid as long as $t(\varepsilon)$ does not change significantly within the bands so that ex-

pansion of a single scattering WP into one transmitted and one reflected bulk WP is satisfactory. If this is not the case the scattering WPs, while still containing exactly one electron will be more delocalized and the contribution to the current at x_0 will have significant contributions from many consecutive bulk WPs. Clearly, under such circumstances one can gain physical insight by simply introducing several narrower energy bands to suppress the energy variation of transmission amplitude within these bands, so that the nonlinear character becomes apparent.

This discussion also indicates that the WPB representation can be used not only as a means to understand the physics behind non-equilibrium transport, but also as a method to perform numerical *ab initio* time-dependent simulations within the TDDFT framework, i.e. accounting for time-dependent self-consistent field. The time-evolution of the bulk WP as they enter the scattering region needs to be done numerically, but as soon as the scattered WP leaves this region, by expanding it into few bulk WPs one can perform its time evolution algebraically in a closed form. The density, current density or any other many-electron property is obtained by summing contributions from all stroboscopic images of the propagated WP. The implementation of this scheme will be reported elsewhere[16].

We also mention that within the WPB-based picture, the memory-loss theorem[13,17], stating the independence of the steady state on the transient changes in external potential, is very easy to understand: from the moment when the potential attains its long-time static form, it takes only a finite time until the WPs experiencing the transient potential leave the scatterer into the bulk, never to return. After that the occupancies of all the WPs inside this region are determined by the scattering of the bulk WPs within the long-time static potential.

Edge-induced spin Hall effect. It has been recently shown that the interplay between nonzero Rashba-Bytchkov spin-orbit (SO) coupling, the scattering off the edge and nonzero electric current along this edge leads to a universal spin polarization localized close to the edge of the 2D gas in GaAs quantum wells[18,19]. In parallel, several other authors[20,21,22] considered the spin-orbit (SO) coupling due to nonzero gradient in potential in-plane,

$$V_{SO} = -\alpha_E \left[\hat{\sigma} \times \nabla V(\mathbf{r})\right] \cdot \hat{\mathbf{p}}, \tag{7}$$

where α_E is the strength of the SO coupling, $\hat{\sigma}$ is the operator of spin, $V(\boldsymbol{r})$ is the confining potential at the edge and $\hat{\mathbf{p}}$ the momentum operator[27]. The edge-SO scattering, analogous to the mechanism behind impurity scattering in the bulk of the 2D gas, seems to lead to effects similar to the Rashba-Bytchkov mechanism.

Both of these effects can be understood and analyzed within the WPB description, but here we concentrate on the edge-SO scattering. We consider a 2D electron gas confined in the $xy(x>0)$ half-plane, with its edge being described by a model potential $V(\boldsymbol{r}) = W\theta(-x)$ where θ is the step function. This model is appropriate for typical doping densities $n \sim 10^{22}\mathrm{cm}^{-2}$ where the Fermi wavelength $\lambda_F \sim 20\mathrm{nm}$ is much larger than atomic spacing, principally determining the abruptness of the edge. The current is imposed in the y direction. Fourier transforming $y \to k_y$, the SO term takes the form $V_{SO} = \alpha_E \hat{\sigma}_z W \delta(x) k_y$, i.e. electrons with up and down spins in the z direction experience different scattering potential at the edge. For each k_y we construct a WP, localized in the x direction and constructed from the eigenstates of a bulk 2D electron gas. If we time-propagate an initial WPs with an average k_x pointing towards the edge and identical for both up and down spin states (left-going WP), the reflected WPs for up and down spins will have two different phase shifts $\phi_{\uparrow/\downarrow}$, and hence a *mutual spatial shift* l_S with respect to one other. For the model described here the shift is

$$l_S = \langle \frac{d}{dk_x}(\phi_\uparrow - \phi_\downarrow)\rangle = -4\alpha_E - 8(2W - \langle e\rangle)\alpha_E^3 + \mathscr{O}(\alpha_E^4), \tag{8}$$

where the averaging is over the energy band of the considered WP and $e = (k_x^2 + k_y^2)/2$. We know that WPs separated by the time-step τ are orthogonal and we may place one electron in each WP. The non-equilibrium situation can be set in the standard fashion: occupying the WPs with $k_y > 0$ up to $E_F + \Delta V$ and those WPs with $k_y < 0$ only up to E_F. Deep inside the 2D bulk this WPs' shift will not contribute to any spin polarization because a series of occupied WPs within each band gives homogeneous density. However, since the up- and down-spin WPs are shifted, this shift must be directly related to the spin accumulation close to the edge so that to first order in α_E

$$n_\uparrow - n_\downarrow \sim \int_{occ} \frac{dk_y}{2\pi} l_S n(k_y) \sim -\frac{2\alpha_E}{\pi^2}\sqrt{2E_F}\Delta V, \tag{9}$$

where $n(k_y) = \sqrt{2E_F - k_y^2}/\pi$ is the number of initial WPs with momentum k_y. The dependence on the magnitude of the confinement, W comes only in the 3th order, which follows from Eq. 8 and 9

$$\frac{d}{dW}(n_\uparrow - n_\downarrow) = -\frac{8\alpha_E^3}{\pi^2}\sqrt{2E_F}\Delta V, \tag{10}$$

and hence the actual magnitude of the confinement potential is rather unimportant. Both of the results, Eqs. 9 and 10, agree very well with more involved and exact Green's function based treatments which will be reported elsewhere[23], and demonstrate the usefulness of the WPB concept not only for qualitative but also for reliable quantitative estimates.

It is interesting to compare the edge-SO scattering with the Rashba-Bytchov mechanism. The latter gives[19] $n_\uparrow - n_\downarrow = -\alpha_R^2 (2E_F)^{-3/2} \Delta V/(12\pi^2)$, where α_R is the strength of the Rashba coupling; in the 2D GaAs systems it attains values[24] $\alpha_R \sim 1.8 \times 10^{-10}$eV cm $= 1.55 \times 10^{-2}$a.u.*. On the other hand, the estimates for α_E in GaAs quantum wells give[25] $\alpha_E \sim 5.3\mathring{A}^2 = 5.53 \times 10^{-4}$a.u.*. The smallness of both α_E and α_R justifies the lowest order expansions used above. Finally, taking for the Fermi energy, $E_F = 36$meV$= 3.01$a.u.* corresponding to densities $n \sim 10^{12}$cm^{-2} we find that the Rasba-mechanism is three orders of magnitude smaller than the edge spin-orbit scattering. In principle this might change at very low densities since the Rashba-mechanism increases while the edge SO scattering decreases with decreasing the Fermi energy (or density) but for such low densities the behavior will be dominated by localization and interactions effects.

In conclusion, our stroboscopic wavepacket basis permits both physical understanding and quantitative predictions to be obtained for a variety of non-equilibrium processes in which an extended system of electrons is subject to time-evolution while being coupled to bulk reservoirs. The stroboscopic construction permits the time-evolution of the system to be described straightforwardly, while the energy-localisation of the wavepackets within precise energy bands ensures that the Pauli principle is properly respected in coupling to the reservoirs.

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