

Uniform electron gas in the presence of space-time periodic potentials: Floquet-Bloch and linear-response theory

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Nonequilibrium quantum physics greatly simplifies in the case of time-periodic Hamiltonians, since Floquet theory provides an analog to Bloch's theorem in the time domain. Still, the formal properties of Floquet many-body theory remain underexplored. Here, we study what happens to the uniform electron gas when a space-time periodic potential of arbitrary strength is applied, which leads to band splitting. The case of a potential traveling at constant speed is special, since the problem can be made time independent by transforming to a comoving frame. We perform linear-response theory, in the sense that we apply an additional perturbatively small but nonperiodic probing field, for which we illustrate the analogy of Fermi's golden rule and the photoemission spectrum of a many-electron system. As in the equilibrium case, the latter is related to the spectral function which is positive definite. We also analyze the parameter dependence of the controllable photoemission spectra by virtue of Floquet-Bloch engineering.

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I. INTRODUCTION

The dynamics of quantum many-particle systems under time-dependent external fields is one of the most active fields of research in chemistry and condensed matter physics in the last few decades, both experimentally [1,2] and theoretically [3–5]. A wide variety of new phenomena not accessible in systems in equilibrium reveal themselves in the presence of time-dependent fields. An intriguing example are photo-induced phase transitions [6,7]. The possibility of controlling the phase of matter and changing the electronic [8] as well as magnetic [9–11] properties of a material using a time-dependent external field is rather appealing, especially in the context of ultrafast (femtosecond) phenomena that access the intrinsic timescales of the electrons in a solid.

A particular type of time-dependent external field of great interest is a time-periodic one, since the discrete time translation symmetry allows a treatment via Floquet theory. These fields make it possible to perform Floquet design, in which quantum systems are subjected to a chosen external drive to achieve certain desired properties such as topological phases [11–18]. Despite the ubiquity of periodically driven quantum systems, relatively little is known about the fundamental aspects of Floquet theory, especially in the many-body context. Only very recently the positivity of the spectral functions

extracted from the retarded Floquet Green's function was rigorously established [19].

In this article, we are interested in external fields which have a combined spatial and temporal periodic structure, which makes it possible to do Floquet-Bloch engineering [20]. More specifically, we consider (linear combinations of) traveling wave potential(s), where the space- and time dependence are intertwined. We consider the nonrelativistic limit, in the sense that the traveling wave potential has a velocity that is much smaller than the speed of light. The traveling wave setup can be contrasted with the application of long-wavelength light to a periodic structure, where the Hamiltonian contains separate time-periodic and space-periodic parts, which has been studied in several previous works [21–24].

A potential realization of such a traveling wave potential is in trapped cold atom systems, where optical lattices can be induced via external laser beams. Along the same line, optical gratings provide a way to introduce large-scale space-periodic potentials [25] in solid state physics. Periodic, low-frequency modulation of the optical set-up in these experiments can be used to create the kind of space-time periodic potential considered here.

In this work, we study the noninteracting fermion (electron) gas for simplicity, to get a feeling for the basic physics of the spatiotemporal periodicity. This study can form the basis for similar studies of lattice Hamiltonians or of interacting systems using, e.g., the *GW* method. Apart from the explicit time-dependent Hamiltonian, our fermion gas is an isolated system, not connected to any leads, bath or reservoir.

To analyze the physics of the system, we use linear-response theory for periodically driven many-electron systems in the wave function and Green's function formalisms [26–29]. We discuss the relations between these formalisms,

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especially in terms of the initial condition. The linear response is with respect to the nonperiodic probing field that is applied *on top of* the space-time periodic potential. For a harmonic perturbation, the corresponding Fermi golden rule for a Floquet system can be used to calculate the photoemission spectra [30–32] and the resulting spectra are related to a component of the Floquet Green's function with positive definite spectra [19]. Thus, the density of states measured in photoemission experiments is identified with the appropriate component of the Floquet Green's function, both in the many-body and noninteracting case.

II. FLOQUET THEORY

A time-periodic Hamiltonian can be treated within Floquet theory, an analog of Bloch theory for a periodic potential in space, and the two can also be combined [23]. We start with a short review of Floquet theory. The one-particle time-dependent Schrödinger equation is given by

$$[\hat{H}_0(r, t) - i\partial_t]\psi(r, t) = 0, \quad (1)$$

with time-periodicity, i.e., $\hat{H}_0(r, t + T) = \hat{H}_0(r, t)$. Here, r denotes space and spin variables, $r = (\mathbf{r}, \sigma)$.

According to Floquet's theorem, solutions to the time-dependent Schrödinger equation with a periodic potential in time have the form

$$\psi_\alpha(r, t) = e^{-i\varepsilon_\alpha t} \phi_\alpha(r, t), \quad (2)$$

where $\phi_\alpha(r, t)$ is periodic in time with period T ,

$$\phi_\alpha(r, t + T) = \phi_\alpha(r, t), \quad (3)$$

and it is an eigenfunction of the Floquet operator

$$\hat{H}_F(r, t) = H_0(r, t) - i\partial_t \quad (4)$$

with eigenvalue ε_α :

$$\hat{H}_F(r, t)\phi_\alpha(r, t) = \varepsilon_\alpha \phi_\alpha(r, t). \quad (5)$$

Here, $\psi_\alpha(r, t)$ and $\phi_\alpha(r, t)$ are called a Floquet state and a Floquet mode, respectively. Equation (2) implies that

$$\psi_\alpha(r, t + T) = e^{-i\varepsilon_\alpha T} \psi_\alpha(r, t), \quad (6)$$

which is the analog of the Bloch theorem for solutions to the Hamiltonian of a periodic crystal and ε_α is the analog of the crystal momentum, whereas T plays the role of the primitive translation vector in space. From the group theory point of view, $\exp(-i\varepsilon_\alpha T)$ can be regarded as a one-dimensional irreducible representation of the element T of the Abelian time translation group.

It is clear that if $\phi_\alpha(r, t)$ is a Floquet mode, then

$$\phi_{n\alpha}(r, t) = \phi_\alpha(r, t)e^{in\Omega t}, \quad (7)$$

where $\Omega = 2\pi/T$, is also a Floquet mode with eigenvalue

$$\varepsilon_{n\alpha} = \varepsilon_\alpha + n\Omega. \quad (8)$$

The corresponding Floquet state $\psi_{n\alpha}(r, t)$ is identical to $\psi_\alpha(r, t)$:

$$\psi_{n\alpha}(r, t) = e^{-i\varepsilon_{n\alpha}t} \phi_{n\alpha}(r, t) = e^{-i\varepsilon_\alpha t} \phi_\alpha(r, t) = \psi_\alpha(r, t). \quad (9)$$

The property in Eq. (8) allows us to restrict ε_α as follows:

$$-\frac{\Omega}{2} \leq \varepsilon_\alpha < \frac{\Omega}{2}. \quad (10)$$

The segment $[-\frac{\Omega}{2}, \frac{\Omega}{2}]$ is the analog of the first Brillouin zone in a periodic crystal. We have considered a one-particle Floquet system, but the same properties are also valid in a many-particle Floquet system.

A. Photoemission spectra in Floquet systems

We briefly review Fermi's golden rule for photoemission in Floquet systems, more details are provided in Appendixes A and B and the literature [19,30].

In the presence of an electromagnetic field, the electron momentum operator $\hat{\mathbf{p}}$ is replaced by [33] $\hat{\mathbf{p}} - (e/c)\mathbf{A}(\hat{\mathbf{r}}, t)$ so that the kinetic energy becomes

$$\begin{aligned} & \frac{1}{2m}[\hat{\mathbf{p}} - (e/c)\mathbf{A}(\hat{\mathbf{r}}, t)]^2 \\ &= \frac{\hat{\mathbf{p}}^2}{2m} - \frac{e}{2mc}[\hat{\mathbf{p}} \cdot \mathbf{A}(\hat{\mathbf{r}}, t) + \mathbf{A}(\hat{\mathbf{r}}, t) \cdot \hat{\mathbf{p}}] + \left(\frac{e}{2mc}\right)^2 \mathbf{A}^2(\hat{\mathbf{r}}, t). \end{aligned} \quad (11)$$

The last term is usually neglected since it is proportional to $1/c^2$ and involves two-photon processes in first-order perturbation theory. It is assumed that the vector potential represents a monochromatic field

$$\begin{aligned} \mathbf{A} &= 2A_0\hat{\varepsilon} \cos\left(\frac{\omega}{c}\hat{\mathbf{n}} \cdot \mathbf{r} - \omega t\right) \\ &= A_0\hat{\varepsilon}\left[e^{i(\frac{\omega}{c}\hat{\mathbf{n}} \cdot \mathbf{r} - \omega t)} + e^{-i(\frac{\omega}{c}\hat{\mathbf{n}} \cdot \mathbf{r} - \omega t)}\right]. \end{aligned} \quad (12)$$

$\hat{\varepsilon}$ is the light polarization and $\hat{\mathbf{n}}$ is the propagation direction, and they are perpendicular to each other. Using the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ and treating

$$-\frac{e}{2mc}(\hat{\mathbf{p}} \cdot \hat{\mathbf{A}} + \hat{\mathbf{A}} \cdot \hat{\mathbf{p}}) = -\frac{e}{mc}\hat{\mathbf{A}} \cdot \hat{\mathbf{p}} \quad (13)$$

as a perturbation representing the coupling between the photon and the electron, the Fermi golden rule from the previous section can be directly applied. One identifies

$$\hat{V} = -\frac{eA_0}{mc}e^{i\frac{\omega}{c}\hat{\mathbf{n}} \cdot \hat{\mathbf{r}}} \hat{\varepsilon} \cdot \hat{\mathbf{p}}. \quad (14)$$

In the occupation number representation,

$$\hat{V}(t) = \sum_{ij} (V_{ij}e^{i\omega t} + V_{ij}^*e^{-i\omega t})\hat{c}_i^\dagger \hat{c}_j. \quad (15)$$

In a photoemission experiment, an electron is removed from an N -electron system, which in the present case is a Floquet system. The calculation of the photoemission spectrum is greatly simplified under the so-called sudden approximation [34–36] in which the photoelectron is assumed to be suddenly removed from the system and completely decoupled from the remaining $(N-1)$ -electron system. This assumption is valid when the kinetic energy of the photoelectron is large compared to its binding energy in the solid.

Let the initial state be a Floquet mode $|\Phi_\alpha(t_0)\rangle$. Note that the Greek alphabet is used to denote many-electron states whereas Roman letters are used to denote one-particle base functions. Within the sudden approximation, the Floquet

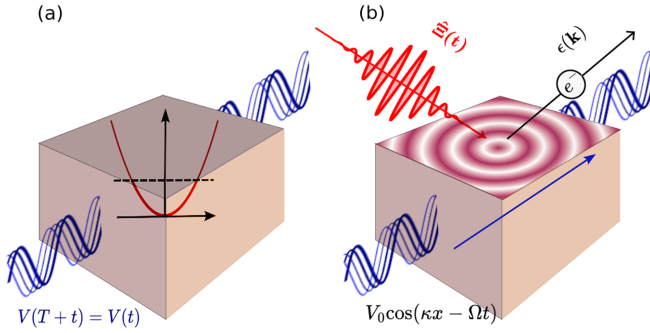


FIG. 1. Schematic diagram of the formalism followed in this paper. (a) The system is initially prepared in a Floquet state with an external periodic driving field. (b) On top of that we apply a probing field that causes further electronic transitions or emission.

mode $|\Phi_\beta(t)\rangle$, which is coupled by the photon field to the initial state, can be written as

$$|\Phi_\beta(t)\rangle = \hat{c}_k^\dagger |\Phi_\gamma^{N-1}(t)\rangle \quad (16)$$

in which $\hat{c}_k^\dagger$ represents the photoelectron with momentum $k = (\mathbf{k}, \sigma)$ and $|\Phi_\gamma^{N-1}(t)\rangle$ is an $(N-1)$ -electron Floquet mode. It is evident that $\hat{c}_i^\dagger$ in Eq. (15) must be equal to $\hat{c}_k^\dagger$ for otherwise the matrix element would vanish. The transition matrix elements corresponding to an absorption process is then

$$\langle \Phi_\gamma^{N-1}(t_1) | \sum_j V_{kj}^* \hat{c}_j | \Phi_\alpha(t_1) \rangle = \sum_m f_m^{k\alpha\gamma} e^{im\Omega t_1}, \quad (17)$$

and the operator $\hat{\Xi}^\dagger$ in Eq. (C5) can be identified as

$$\hat{\Xi}^\dagger = \sum_j V_{kj}^* \hat{c}_j. \quad (18)$$

The Fermi golden rule for absorption in Eq. (C16) can now be applied to calculate the photocurrent with energy ϵ_k , the kinetic energy of the outgoing photoelectron, yielding

$$I(\epsilon_k) \propto \sum_{\gamma m} |f_m^{k\alpha\gamma}|^2 \delta[\omega - \epsilon_k - m\Omega - (E_\gamma^{N-1} - E_\alpha)]. \quad (19)$$

The right-hand side of this equation, and thus also the photocurrent, is proportional to the imaginary part of the $l=0$ component of the Floquet Green's function [19]. In general, both the initial and final states should be weighted by taking into account the matrix element of the dipole operator between these two states.

III. NONINTERACTING ELECTRON GAS IN TRAVELING WAVE POTENTIAL

Here, we consider the noninteracting electron gas in the presence of a superposition of space-time periodic traveling wave potentials of the form $V(x, t) = \sum_\alpha V_\alpha \cos(n_\alpha \kappa x - m_\alpha \Omega t)$, with n_α and m_α integers, as illustrated by the blue curve in Fig. 1. Throughout, we are assuming the nonrelativistic limit $\frac{n_\alpha \kappa}{m_\alpha \Omega} = v_\alpha \ll c$. Since the potential is space-time-periodic, we can apply the Floquet-Bloch formalism to solve the problem. In the traveling wave potential, space and time are intrinsically intertwined, which means that the situation is somewhat different from a Hamiltonian which

is the sum of a space-periodic and a time-periodic part, which is frequently considered in the literature [23].

A. Monochromatic potential

The situation is particularly simple for a monochromatic potential, $V(x, t) = V_0 \cos(\kappa x - \Omega t)$, because there is an alternative solution using a transformation to a comoving frame, in which the potential becomes time-independent and is solved without Floquet using the traditional methods of band theory. This alternative solution makes it a suitable test case for Floquet approaches. We work it out in detail in the original frame here, and in the comoving frame in Sec. III B. In fact, such a transformation to a comoving frame can be used for any linear combination of traveling wave potentials $\sum_\alpha V_\alpha \cos(n_\alpha \kappa x - m_\alpha \Omega t)$ which moves at a single velocity, $v = n_\alpha \Omega / m_\alpha \kappa$ independent of α .

To be more explicit, we start with the well-known solution of a one-dimensional particle with mass m_e in a box of length L with periodic boundary conditions, using units of $\hbar = 1$. The time-independent Schrödinger equation of the free particle $E\psi(x) = -\frac{1}{2m_e} \frac{d^2\psi(x)}{dx^2}$ has plane-wave solutions $\psi(x) = \frac{1}{\sqrt{L}} \exp(ikx)$ with energy $E = k^2/2m_e$ and quantization condition $k = nK$, with $n \in \mathbb{Z}$ and $K = 2\pi/L$.

Now, we apply the space-time-periodic potential $V(x, t) = V_0 \cos(\kappa x - \Omega t)$, with the constraint $\kappa L = 2\pi v$, $v \in \mathbb{Z}$ so that the potential and the box size match. The Floquet-Schrödinger equation is

$$\hat{H}_F = -\frac{1}{2m_e} \frac{\partial^2}{\partial x^2} + V_0 \cos(\kappa x - \Omega t) - i \frac{\partial}{\partial t}, \quad (20)$$

$$\hat{H}_F \phi_\alpha(x, t) = \epsilon_\alpha \phi_\alpha(x, t),$$

where $\phi_\alpha(x, t)$ is periodic in time with period $T = 2\pi/\Omega$, and we can restrict the eigenvalues ϵ_α to the first Floquet Brillouin zone. The space-time-periodic solution can be Fourier-decomposed as

$$\phi_\alpha(x, t) = \sum_{n,m} c_{\omega,k}^\alpha \exp(i\omega t) \exp(ikx),$$

where $c_{\omega,k}^\alpha$ is the Fourier coefficient of the (ω, k) component and $\omega = m\Omega$ and $k = nK$ are restricted to discrete values. Note that m is a Floquet index while m_e is the electron mass.

With this ansatz,

$$\begin{aligned} \hat{H}_F \phi_\alpha(x, t) &= \sum_{k,\omega} \left(\omega + \frac{k^2}{2m_e} \right) c_{\omega,k}^\alpha \exp(i\omega t) \exp(ikx) \\ &+ \sum_{\omega,k} \frac{V_0}{2} c_{\omega,k}^\alpha \exp(i(k+\kappa)x) \exp(i(\omega-\Omega)t) \\ &+ \sum_{\omega,k} \frac{V_0}{2} c_{\omega,k}^\alpha \exp(i(k-\kappa)x) \exp(i(\omega+\Omega)t) \\ &= \epsilon_\alpha \sum_{\omega,k} c_{\omega,k}^\alpha \exp(i\omega t) \exp(ikx). \end{aligned} \quad (21)$$

Written as a supermatrix in (ω, k) , (ω', k') , $\hat{H}_F$ has diagonal components $\frac{k^2}{2m_e} + m\Omega$, and off-diagonal components $\frac{V_0}{2}$ connecting (ω, k) with $(\omega + \Omega, k - \kappa)$ and $(\omega - \Omega, k + \kappa)$.

In other words, an electron can absorb or emit quanta of combined energy and momentum. Eigenvalues and eigenvectors of the supermatrix equation can be found numerically and lead to the photoemission spectra discussed below. At the zone boundary, only two modes contribute and the problem can be solved analytically to find the magnitude of the band splitting, see Appendix D.

B. Comoving frame

Our choice of potential becomes time independent in a comoving frame, which allows for a solution without Floquet theory. We introduce the comoving coordinates (y, τ) with $y(x, t) = x - \frac{\Omega}{\kappa}t$ and $\tau(x, t) = t$, i.e., $x(y, \tau) = y + \frac{\Omega}{\kappa}\tau$, and the function $\tilde{\phi}$ so that $\tilde{\phi}(y, \tau) = \phi(x(y, \tau), t(y, \tau))$, where $\phi(x, t)$ is a solution to the time-dependent Schrödinger equation in the original reference frame. Then,

$$\frac{\partial \tilde{\phi}}{\partial y} = \frac{\partial \phi}{\partial x} \frac{\partial x}{\partial y} + \frac{\partial \phi}{\partial t} \frac{\partial t}{\partial y} = \frac{\partial \phi}{\partial x}, \quad (22)$$

$$\frac{\partial \tilde{\phi}}{\partial \tau} = \frac{\partial \phi}{\partial x} \frac{\partial x}{\partial \tau} + \frac{\partial \phi}{\partial t} \frac{\partial t}{\partial \tau} = \frac{\partial \phi}{\partial x} \frac{\Omega}{\kappa} + \frac{\partial \phi}{\partial t}, \quad (23)$$

$$\frac{\partial \phi}{\partial t} = \frac{\partial \tilde{\phi}}{\partial \tau} - \frac{\Omega}{\kappa} \frac{\partial \tilde{\phi}}{\partial y}, \quad (24)$$

$$\begin{aligned} \frac{\partial^2 \tilde{\phi}}{\partial y^2} &= \frac{\partial^2 \phi}{\partial x^2} \left(\frac{\partial x}{\partial y} \right)^2 + \frac{\partial^2 \phi}{\partial t^2} \left(\frac{\partial t}{\partial y} \right)^2 + 2 \frac{\partial^2 \phi}{\partial t \partial x} \frac{\partial t}{\partial y} \frac{\partial x}{\partial y} \\ &= \frac{\partial^2 \phi}{\partial x^2}. \end{aligned} \quad (25)$$

Thus, the differential equation transforms as

$$\begin{aligned} \epsilon_\alpha \tilde{\phi}_\alpha(y, \tau) &= \left(-\frac{1}{2m_e} \frac{\partial^2}{\partial y^2} + V_0 \cos(\kappa y) - i \frac{\partial}{\partial \tau} + i \frac{\Omega}{\kappa} \frac{\partial}{\partial y} \right) \\ &\times \tilde{\phi}_\alpha(y, \tau). \end{aligned} \quad (26)$$

In the new frequency-momentum space, with the momentum conjugate to y denoted by k_y , the Floquet-Schrödinger equation is

$$\begin{aligned} \left(\frac{k_y^2}{2m_e} - \frac{\Omega}{\kappa} k_y + m\Omega - \epsilon_\alpha \right) c_{m, k_y}^\alpha + \frac{V_0}{2} c_{m, k_y + \kappa}^\alpha + \frac{V_0}{2} c_{m, k_y - \kappa}^\alpha \\ = 0. \end{aligned} \quad (27)$$

This equation is diagonal in m , which reflects the time-independence of the problem in this reference frame, so we can drop the m label everywhere and go back to regular energies $\epsilon_\alpha - m\Omega = E_\alpha$, i.e.,

$$\left(\frac{k_y^2}{2m_e} - \frac{\Omega}{\kappa} k_y - E_\alpha \right) c_{k_y}^\alpha + \frac{V_0}{2} c_{k_y + \kappa}^\alpha + \frac{V_0}{2} c_{k_y - \kappa}^\alpha = 0. \quad (28)$$

At this point, the only difference with the usual particle in a cosine potential is the form of the kinetic energy: In terms of the semiclassical interpretation, a particle with $k_y = 0$ is standing still in the comoving frame but is moving with velocity Ω/κ in the original frame, giving it a finite kinetic energy. Thus, the initial band structure before applying the potential is a parabola centered away from $k_y = 0$.

C. Many-electron wave function

We have now found the single-particle eigenfunctions of the Schrödinger equation in both frames. For the noninteracting electron gas, the general N -particle solutions are Slater determinants of single-particle solutions with N occupied orbitals, whose energy is the sum of the single-particle energies of the occupied states.

A particular solution of the Schrödinger equation is found when the many-particle wave function $\psi(t_0)$ at any time t_0 is inserted as a boundary condition, by decomposing $\psi(t_0)$ into Slater determinants and time-evolving them separately. Similarly, if the system is not in a pure state but in a statistical ensemble $\rho(t_0)$ at t_0 , decomposition into an ensemble of Slater determinants gives the solution to the von Neumann equation of motion. This solution strategy works both in the original and in the comoving frame. We note that the total number of electrons is a conserved quantity and is therefore determined by the number of electrons at t_0 .

Instead of a boundary condition at t_0 , another way to find a particular solution is via the connection to a reservoir, in which case the properties of the reservoir (temperature, etc.) determine the properties of the solution. In particular, for the time-independent Schrödinger equation, there is the ground state ($T = 0$) solution at fixed electron number, which minimizes the total energy. In the Floquet picture, because energy is only defined modulo Ω , it is not possible to identify a ground state in a similar way. Still, in the case where the time-periodic potential is small in magnitude, it is possible to consider the ground state without potential and to use this as the boundary condition determining the particular solution of the differential equation, but it should be stressed that this is a somewhat arbitrary choice.

D. Green's function formalism

Green's functions form an alternative to the wave function formalism and a natural starting point for many-body perturbation theory approaches such as *GW*. The time-ordered and the retarded Green's functions are defined by [37]

$$iG^{\text{TO}}(rt, r't') = \langle \Psi_0 | \mathcal{T} \hat{\psi}_0(rt) \hat{\psi}_0^\dagger(r't') | \Psi_0 \rangle, \quad (29)$$

$$iG^{\text{R}}(rt, r't') = \theta(t - t') \langle \Psi_0 | \{ \hat{\psi}(rt), \hat{\psi}^\dagger(r't') \} | \Psi_0 \rangle. \quad (30)$$

Here, $\mathcal{T}$ denotes the time-ordering of the operators $\hat{\psi}_0, \hat{\psi}_0^\dagger$. In the presence of an external space-time periodic potential $V(r, t) = \frac{1}{2} \sum_{mn} V_{mn} e^{i(m\kappa r - n\Omega t)}$, the Floquet Green's function is obtained by solving this Dyson-like equation

$$\begin{aligned} \text{---} \xrightarrow{G} \text{---} &= \text{---} \xrightarrow{G^0} \text{---} + \text{---} \xrightarrow{G^0} \text{---} \overset{\times}{\text{---}} \xrightarrow{V} \text{---} \xrightarrow{G} \text{---} \end{aligned} \quad (31)$$

$$\begin{aligned} G(rt, r't') &= G^0(rt, r't') + \int dr'' dt'' G^0(rt, r''t'') V(r''t'') \\ &\times G(r''t'', r't'). \end{aligned} \quad (32)$$

Here, G^0 is the solution without time-dependent potential. The time-ordered and retarded Green's functions in Eqs. (29) and

(30) satisfy this Dyson-like equation individually.¹ In terms of the Bloch-Floquet modes the Dyson-like equation becomes

$$G_{m,m',n,n'}(k, \omega) = G_{m,m',n,n'}^0(k, \omega) \delta_{m,m'} \delta_{n,n'} + \sum_{j,l} G_{m,m,n,n}^0(k, \omega) V_{m-l,n-j} G_{l,m',j,n'}(k, \omega). \quad (33)$$

The Bloch-Floquet modes of the Green's function are defined as

$$G_{m,m',n,n'}(k, \omega) = \frac{1}{(2\pi)^4} \int \left[dt dt' e^{i(\omega+n\Omega)t} \left(\int dr dr' \times e^{i(k+m\kappa)r} G(r, r', t, t') e^{-i(k+m'\kappa)r'} \right) \times e^{-i(\omega+n'\Omega)t'} \right].$$

In Eqs. (33) and (34), k and ω are restricted to the first Brillouin zone. Tracing out the Bloch and Floquet indices leaves an object depending on a single frequency and momentum, which corresponds to taking the average over $t' + t$ and $r' + r$ while Fourier transforming with respect to $t - t'$ and $r - r'$,

$$G(k, \omega) = \sum_{mm'} \sum_{nn'} G_{mm'nn'}(k, \omega). \quad (34)$$

In the Floquet Green's function formalism, a Green's function G^0 that is the solution for a system with a time-independent Hamiltonian is chosen as the starting point and the (still non-interacting) Floquet Green's function is obtained by solving the Dyson-like equation. The choice of G^0 determines the final G . The G^0 corresponding to the ground state of the system without time-dependent potential is a natural choice, but not necessarily the only relevant choice. Other options include finite-temperature or nonequilibrium solutions of system without time-dependent potential. The impact of the choice of G^0 is discussed in more detail in the Results section.

In terms of the Floquet-Bloch modes, the retarded and time-ordered Green's function of the time-independent non-interacting electron gas at zero temperature are

$$(G^R)^0_{mmnn}(\omega, k) = \frac{1}{\omega + n\Omega - \epsilon(k + m\kappa) + i\eta} \quad (35)$$

$$(G^{TO})^0_{mmnn}(\omega, k) = \frac{1}{\omega + n\Omega - \epsilon(k + m\kappa) + i\eta_{mk}}, \quad (36)$$

where $\epsilon(k)$ is the single particle energy with momentum k , η is a small imaginary constant and $\eta_{mk} \equiv \eta \operatorname{sgn}(\epsilon(k + m\kappa))$. Note that the Green's function is diagonal in the Floquet-Bloch indices m, n . The result at zero temperature can be generalized, for any given electronic occupation function

¹For a self-energy, the Dyson equation is a matrix equation in Keldysh space, which means that the retarded, advanced and Keldysh components are connected in principle. However, specifically for a potential, the Keldysh component $V^K = 0$ so that the Dyson equation for the retarded component decouples, see Eq. (2.31) in Ref. [37].

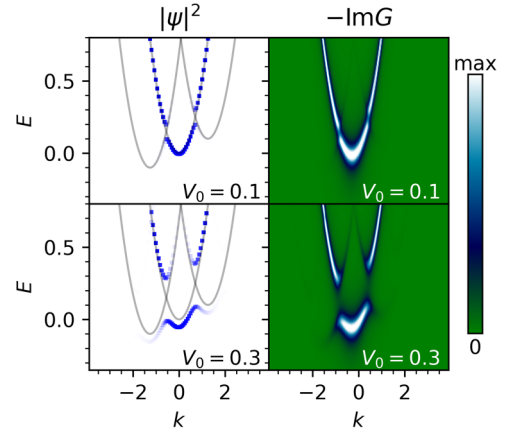


FIG. 2. Solutions for a particle in a box exposed to a traveling wave potential $V_0 \cos(\kappa x - \Omega t)$ for two values of V_0 (top, bottom) in the wave function and Green's function formalism (left, right). In all panels, $\kappa = 20 \frac{2\pi}{L} \approx 1.26$ and $\Omega = 0.1$ determine the spatiotemporal structure of the potential.

$f(\epsilon)$, the time-ordered Green's function is

$$(G^{TO})^0_{mmnn}(\omega, k) = \frac{f(\epsilon)}{\omega + n\Omega - \epsilon(k + m\kappa) - i\eta} \quad (37)$$

$$+ \frac{1 - f(\epsilon)}{\omega + n\Omega - \epsilon(k + m\kappa) + i\eta}. \quad (38)$$

IV. RESULTS

A. Monochromatic wave

Figures 2 and 3 show the Floquet solution of electrons with mass $m_e = 1$ in a box of length $L = 100$ exposed to the space-time periodic potential $V(x, t) = V_0 \cos(\kappa x - \Omega t)$. The simulations are performed using $N_{\text{Floquet}} = 60$, $N_{\text{Bloch}} = 60$.

For the wave function solution (left side in Figs. 2 and 3), solving Eq. (21) gives eigenvalues ϵ_α and eigenvector

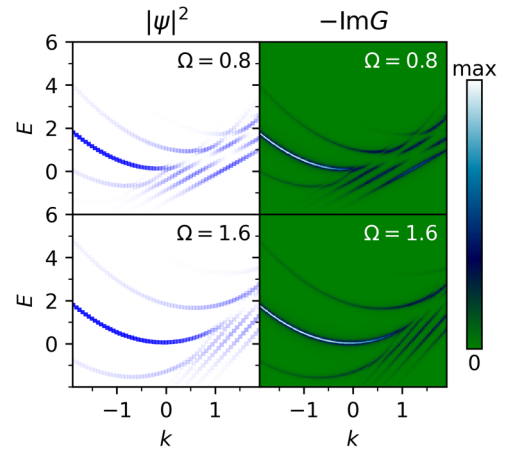


FIG. 3. Solutions for a particle in a box exposed to a traveling wave potential. Here, two different frequencies $\Omega = 0.8$ and $\Omega = 1.6$ are shown (top, bottom), the strength of the potential in the respective simulations is $V_0 = \sqrt{\Omega}$. The wave number $\kappa = 10 \frac{2\pi}{L}$, other parameters are as in Fig. 2. Results for the wave function and Green's function formalism are shown (left, right).

components $c_{m,k}$. We restrict ourselves to the eigenvalues $\epsilon_\alpha \in [0, \Omega]$ in the first Floquet Brillouin zone and map back to the full energy space by plotting a marker with intensity $|c_{m,k}|^2$ at $E = \epsilon_\alpha - m\Omega$. This is similar in spirit to the back-folding to the original Brillouin zone of band structures when working with supercells for charge-density wave or other ordered phases, but now for both momentum and energy. Since these are the eigenfunctions of the (single-particle) Floquet Hamiltonian without applying a boundary condition to obtain a particular solution (with fixed particle number), they only contain information about the spectrum and not about the occupation numbers. For the Green's function solution, the right-hand side of Figs. 2 and 3 shows the retarded component of G , which similarly contains information about the spectrum only. Information about the occupation is contained in $G^<$ and $G^>$ and is discussed in Sec. IV C.

The box size L determines the spacing $\frac{2\pi}{L}$ of the momenta, while Ω and κ determine the size of the Floquet-Bloch Brillouin zone. N_{Floquet} and N_{Bloch} should be chosen large enough to reduce cutoff errors.

Figure 2 shows a “slow” wave, in the sense that $\Omega/\kappa \approx 0.08$ is small compared to the velocity at the edge of the first Bloch Brillouin zone $v(k = \kappa/2) = \frac{\kappa}{2m_e} \approx 0.63$. The gray curves show the bare dispersion $k^2/2m_e$ displaced by $(-\Omega, \kappa)$, i.e., by an integer number of energy-momentum quanta of the potential and the slowness of the wave means that this displacement is mostly horizontal. The result looks similar to the band splitting caused by a time-independent potential (perfectly horizontal displacement of the parabola), with the largest splitting where the parabola cross, close to the Bloch Brillouin zone edges. The magnitude of the potential, $|V_0|$, controls the magnitude of the splitting. One sign of the traveling wave nature of the potential is that the potential breaks time-reversal and spatial inversion symmetry and therefore there is no Kramers degeneracy between $+k$ and $-k$. Thus, the band splitting is different for electrons moving along with the traveling wave versus those moving against it.²

The time dependence becomes more important when we change the frequency Ω , as in Fig. 3 and thereby the velocity of the traveling wave. Spectral weight appears in side bands that follow the main parabola, and band splitting is most prominent where parabolas displaced by integer multiples of $(-\Omega, \kappa)$ cross. Note that the amplitude of the potential in the two panels is scaled so that V_0^2/Ω is constant.

The electronic structures for the wave function and Green's function formalism in both Figs. 2 and 3 are very similar, as they should be. A difference is that the Green's function formalism uses a continuous energy grid and a broadening of delta peaks η , whereas the wave function formalism results in sharp eigenvalues which are plotted as markers.

B. Two traveling waves

A comoving frame solution is no longer possible when there are two traveling waves with different velocity, as in

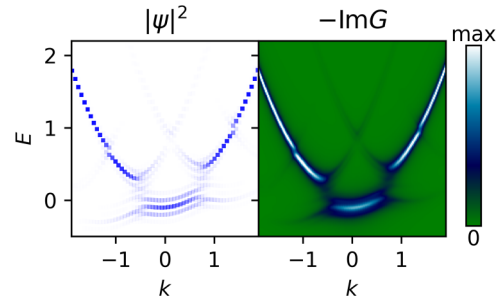


FIG. 4. Solutions for a particle in a box exposed to two traveling wave potentials with different frequency, $\Omega = 0.1$ and $\Omega = 0.2$, both with $V_0 = 0.3$, $\kappa = 20\frac{2\pi}{L}$, i.e., similar to Fig. 2. By emitting and absorbing one quantum from each potential, there is net transfer of energy with net transfer of momentum, so side-bands which are shifted purely vertically appear.

Fig. 4. Both waves have the same wave vector κ , but a different frequency Ω , which makes it possible to absorb or emit a combination of quanta with net energy transfer without net momentum transfer. This leads to the formation vertically shifted side bands, in addition to the diagonally shifted side bands visible in the previous figures. Again, the wave function and Green's function formalism show essentially the same spectra, although the broadening in the Green's function formalism is starting to make it challenging to resolve the individual bands.

C. Photoemission spectra

In the Green's function formalism, the electronic structure can be divided into a direct photoemission and an inverse photoemission part, corresponding to $G^<$ and $G^>$.

$$G^>(rt, r't') = -i \langle \hat{\psi}(rt) \hat{\psi}^\dagger(r't') \rangle \quad (39)$$

$$G^<(rt, r't') = i \langle \hat{\psi}^\dagger(r't') \hat{\psi}(rt) \rangle. \quad (40)$$

They are related to the time-ordered Green's function by

$$G^T(rt, r't') = \theta(t - t')G^>(rt, r't') + \theta(t' - t)G^<(rt, r't'). \quad (41)$$

For a time-independent noninteracting system at zero temperature, the Fermi level cleanly cuts the electronic structure into these two parts. In equilibrium at finite temperature, the Fermi-Dirac occupation function leads to some smearing of both across the Fermi level, on an energy scale $k_B T$ which is usually small compared to the electronic energy scales ($k_B T_{\text{room}} \approx 26 \text{ meV}$). In the Floquet-driven system, on the other hand, the electrons can absorb quanta of energy from the external potential, leading to changes in the occupation numbers. The split between direct and inverse photoemission is therefore not perfect even if one starts with a ground state G_0 , as is done here.

The band structure as well as the direct and inverse photoemission spectra are shown in Figs. 5 and 6. For small κ , the system is in the Floquet limit [39], with nearly vertically displaced side bands, Fig. 5(a). In this case, the direct and inverse photoemission spectra remain restricted to their own region of momentum space, given by the starting Green's

²Note that this is different in the setup of Ref. [38], where there is a time-independent, space-periodic potential $V(x)$ and a field $\sim x \sin(\Omega t)$ which alternates in preferred direction.

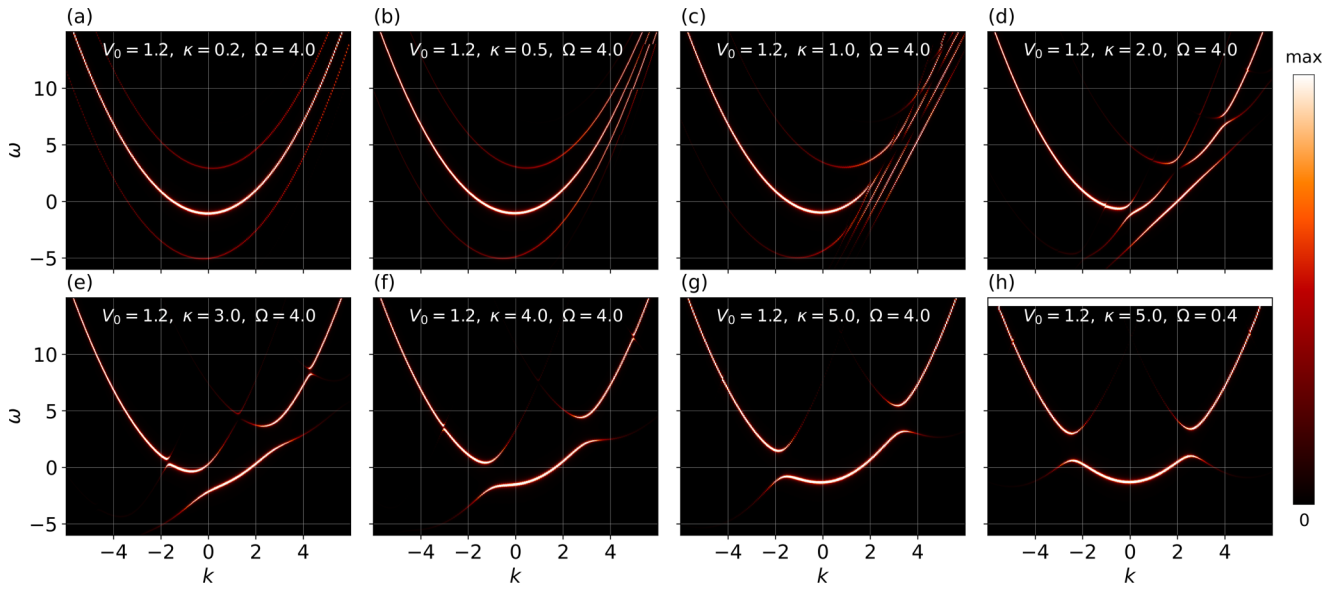


FIG. 5. Band structure of free electron gas under propagating monochromatic external field, derived from the Green's function formalism. Different panels are for different monochromatic waves with a given wave vector κ and frequency Ω .

function G_0 , as shown in Figs. 6(a) and 6(e). The opposite limit of large κ and small Ω leads to the formation of a band gap, Fig. 5(h) in the electronic structure, and some transfer of spectral weight to other Brillouin zones in the direct and inverse photoemission spectra, Figs. 6(d) and 6(h). The reason for this is that momentum is only a good quantum number modulo κ , so the eigenfunctions are linear combinations of modes with $k + n\kappa$, which mixes the occupied and empty states of G_0 .

For intermediate values of κ and Ω , there are substantial parts of (ω, k) space where both direct and inverse photoemission are possible, as is visible in Figs. 6(b), 6(c), 6(f),

and 6(g). This reflects the nonequilibrium nature of this problem.

D. Choice of G_0

To study the influence of the choice of G_0 , we have also performed simulations with a thermal G_0 as the input for the Dyson equation, these are shown in Supplemental Material movie 1 [40]. For the noninteracting system studied here, a different choice of initial occupation numbers leads to changes in the occupations at all times and thus to spectral weight transfer between the direct and inverse photoemission

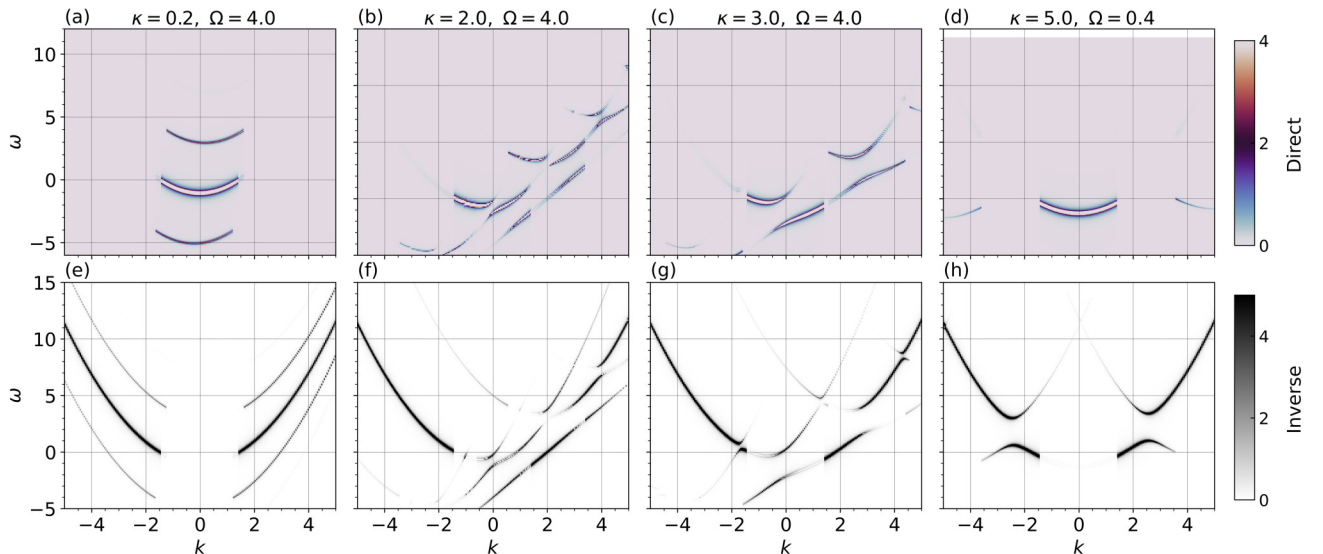


FIG. 6. Photoemission spectra of electron gas under propagating monochromatic electric field. The upper and lower panels represent direct and inverse photoemission spectra, respectively. Different columns represent external fields with different wave vector κ and frequency Ω .

spectra. On the other hand, the spectrum (retarded Green's function) is not affected by the choice of temperature.

V. CONCLUSION

We have applied the Floquet-Bloch formalism to the electron gas in the presence of traveling wave potentials which are periodic in space and time. Both the wave function and the Green's function formalism can be used to describe this kind of system, with consistent results. The Green's function formalism is beneficial as a starting point for the study of interacting systems [41]. In the Floquet theory of closed systems, there is neither a unique ground state nor a reservoir that determines a unique solution. Thus, the outcome of the calculation depends on the "initial" Green's function, G_0 , of the time-independent reference model, for which there is no unique choice. The solution inherits the total particle number from G_0 . A different choice of G_0 leads to spectral weight transfer between the direct and inverse photoemission spectra, as illustrated by our results using finite temperature input.

The linear-response formalism makes it possible to express photoemission spectra in terms of the $l = 0$ component of the imaginary part of the Green's function, which is known to be positive definite. We have analyzed how these photoemission spectra depend on the velocity of the traveling wave potentials, leading to pure Floquet and pure Bloch physics in the limiting cases, with the possibility of Floquet-Bloch engineering in the intermediate regime. Notably, the direction of the traveling wave breaks Kramers degeneracy and therefore reduces the symmetry of the electronic structure.

ACKNOWLEDGMENTS

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DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

APPENDIX A: LINEAR-RESPONSE THEORY IN FLOQUET SYSTEMS

Similar derivations of the response of Floquet systems have been discussed in previous works [17,21,22]. In Sec. B of [17], the authors derive similar expressions using the density matrix approach whereas we use a wave function approach.

The expectation value of an observable associated with an operator $\hat{O}$ as a function of time is given by

$$O(t) = \langle \Psi(t) | \hat{O} | \Psi(t) \rangle = \langle \Psi_F(t) | \hat{O}_F(t) | \Psi_F(t) \rangle. \quad (\text{A1})$$

To first order in the perturbing field

$$\begin{aligned} |\Psi_F(t)\rangle &= \hat{U}_F(t, t_0) |\Psi_F(t_0)\rangle \\ &= \left[1 - i \int_{t_0}^t dt_1 \hat{\Xi}_F(t_1) \right] |\Psi_F(t_0)\rangle, \end{aligned} \quad (\text{A2})$$

yielding

$$\begin{aligned} O(t) &= \langle \Psi_F(t_0) | \hat{O}_F(t) | \Psi_F(t_0) \rangle \\ &\quad - i \int_{t_0}^t dt_1 \langle \Psi_F(t_0) | [\hat{O}_F(t), \hat{\Xi}_F(t_1)] | \Psi_F(t_0) \rangle. \end{aligned} \quad (\text{A3})$$

For an operator that does not depend explicitly on time and assuming that $|\Psi_F(t_0)\rangle$ is a Floquet mode $|\Phi_\alpha(t_0)\rangle$,

$$\begin{aligned} \langle \Psi_F(t_0) | \hat{O}_F(t) | \Psi_F(t_0) \rangle &= \langle \Phi_\alpha(t_0) | \hat{O}_F(t) | \Phi_\alpha(t_0) \rangle \\ &= \langle \Phi_\alpha(t) | \hat{O} | \Phi_\alpha(t) \rangle. \end{aligned} \quad (\text{A4})$$

Consider

$$\begin{aligned} \langle \Phi_\alpha(t_0) | \hat{O}_F(t) \hat{\Xi}_F(t_1) | \Phi_\alpha(t_0) \rangle &= \langle \Phi_\alpha(t_0) | \hat{U}_0(t_0, t) \hat{O} \hat{U}_0(t, t_1) \hat{\Xi}(t_1) \hat{U}_0(t_1, t_0) | \Phi_\alpha(t_0) \rangle \\ &= \langle \Phi_\alpha(t) | \hat{O} \hat{U}_0(t, t_1) \hat{\Xi}(t_1) | \Phi_\alpha(t_1) \rangle e^{-iE_\alpha(t_1-t)} \\ &= \sum_\beta \langle \Phi_\alpha(t) | \hat{O} | \Phi_\beta(t) \rangle \langle \Phi_\beta(t_1) | \hat{\Xi}(t_1) | \Phi_\alpha(t_1) \rangle \\ &\quad \times e^{-i(E_\beta-E_\alpha)(t-t_1)}, \end{aligned} \quad (\text{A5})$$

where Eq. (B6) has been used to obtain the last line. For a perturbing field coupled to the density,

$$\hat{\Xi}(t) = \int dr \varphi(rt) \hat{\rho}(r), \quad (\text{A6})$$

one obtains for the first-order change in the expectation value

$$\begin{aligned} \Delta O(t) &= -i \int dr' \int_{t_0}^t dt_1 \sum_\beta \langle \Phi_\alpha(t) | \hat{O} | \Phi_\beta(t) \rangle \\ &\quad \times \langle \Phi_\beta(t_1) | \hat{\rho}(r') | \Phi_\alpha(t_1) \rangle e^{-i(E_\beta-E_\alpha)(t-t_1)} \varphi(r', t_1) \\ &\quad + i \int dr' \int_{t_0}^t dt_1 \sum_\beta \langle \Phi_\alpha(t_1) | \hat{\rho}(r') | \Phi_\beta(t_1) \rangle \\ &\quad \times \langle \Phi_\beta(t) | \hat{O} | \Phi_\alpha(t) \rangle e^{i(E_\beta-E_\alpha)(t-t_1)} \varphi(r', t_1). \end{aligned} \quad (\text{A7})$$

The retarded linear response can be readily read off from the above expression. Choosing $\hat{O} = \hat{\rho}(r)$ gives the retarded linear density response:

$$\begin{aligned} R^R(rt, r't') &= -i\theta(t-t') \sum_\beta \langle \Phi_\alpha(t) | \hat{\rho}(r) | \Phi_\beta(t) \rangle \\ &\quad \times \langle \Phi_\beta(t') | \hat{\rho}(r') | \Phi_\alpha(t') \rangle e^{-i(E_\beta-E_\alpha)(t-t')} \\ &\quad + i\theta(t-t') \sum_\beta \langle \Phi_\alpha(t') | \hat{\rho}(r') | \Phi_\beta(t') \rangle \\ &\quad \times \langle \Phi_\beta(t) | \hat{\rho}(r) | \Phi_\alpha(t) \rangle e^{i(E_\beta-E_\alpha)(t-t')}. \end{aligned} \quad (\text{A8})$$

This result agrees with a direct evaluation of the retarded density-density correlation function:

$$R^R(rt, r't') = -i\theta(t-t') \langle \Phi_\alpha(t_0) | [\hat{\rho}(rt), \hat{\rho}(r't')] | \Phi_\alpha(t_0) \rangle. \quad (\text{A9})$$

This formula is similar to the *Kubo* formula used in calculation of linear-response properties of a time-independent system, here the initial many-body states $|\Phi_\alpha(t_0)\rangle$ is defined at a particular time t_0 .

APPENDIX B: FLOQUET PICTURE

Sections 2.1 and 2.3 in Ref. [3] and the Supplemental Material of Ref. [19] contain similar derivations.

Let a time-periodic Hamiltonian $\hat{H}_0(t)$ be augmented by an arbitrary external time-dependent perturbing field $\hat{\Xi}(t)$, which is not in general periodic, i.e.,

$$\hat{H}(t) = \hat{H}_0(t) + \hat{\Xi}(t). \quad (\text{B1})$$

Define states in the Floquet picture (interaction picture) as follows:

$$|\Psi_F(t)\rangle = \hat{U}_0(t_0, t)|\Psi(t)\rangle, \quad (\text{B2})$$

$$\hat{U}_0(t, t_0)|\Psi_F(t)\rangle = |\Psi(t)\rangle, \quad (\text{B3})$$

where

$$i\partial_t|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle, \quad (\text{B4})$$

and $\hat{U}_0(t, t_0)$ is the time-evolution operator associated with $\hat{H}_0(t)$, which fulfills the equation of motion

$$i\partial_t\hat{U}_0(t, t_0) = \hat{H}_0(t)\hat{U}_0(t, t_0). \quad (\text{B5})$$

The time-evolution operator of the Floquet system, $\hat{U}_0(t, t_0)$, can be expressed in terms of the Floquet modes as follows [3,19]:

$$\hat{U}_0(t, t_0) = \sum_{\alpha} |\Phi_{\alpha}(t)\rangle e^{-iE_{\alpha}(t-t_0)} \langle\Phi_{\alpha}(t_0)|. \quad (\text{B6})$$

The many-body Floquet modes $\Phi_{\alpha}(t)$ are the eigenvectors of the Floquet Hamiltonian

$$[\hat{H}_0(t) - i\partial_t]|\Phi_{\alpha}(t)\rangle = E_{\alpha}|\Phi_{\alpha}(t)\rangle. \quad (\text{B7})$$

E_{α} are the eigenvalues of the many-body Floquet Hamiltonian or the many-body quasienergy. Operators in the Floquet picture are defined as

$$\hat{O}_F(t) = \hat{U}_0(t_0, t)\hat{O}(t)\hat{U}_0(t, t_0), \quad (\text{B8})$$

where $\hat{O}(t)$ is an operator in the Schrödinger picture.

Taking the time derivative of Eq. (B3) yields

$$(i\partial_t\hat{U}_0(t, t_0))|\Psi_F(t)\rangle + \hat{U}_0(t, t_0)i\partial_t|\Psi_F(t)\rangle = i\partial_t|\Psi(t)\rangle. \quad (\text{B9})$$

Using Eqs. (B6) and (B4) leads to

$$\hat{U}_0(t, t_0)i\partial_t|\Psi_F(t)\rangle = \hat{\Xi}(t)\hat{U}_0(t, t_0)|\Psi_F(t)\rangle. \quad (\text{B10})$$

Applying $\hat{U}_0(t_0, t)$ on both sides of the above equation gives

$$i\partial_t|\Psi_F(t)\rangle = \hat{\Xi}_F(t)|\Psi_F(t)\rangle, \quad (\text{B11})$$

where

$$\hat{\Xi}_F(t) = \hat{U}_0(t_0, t)\hat{\Xi}(t)\hat{U}_0(t, t_0). \quad (\text{B12})$$

Define the time-evolution operator in the Floquet picture as follows:

$$|\Psi_F(t)\rangle = \hat{U}_F(t, t_0)|\Psi_F(t_0)\rangle. \quad (\text{B13})$$

From Eq. (B11) one obtains

$$i\partial_t\hat{U}_F(t, t_0) = \hat{\Xi}_F(t)\hat{U}_F(t, t_0), \quad (\text{B14})$$

with the formal solution

$$\hat{U}_F(t, t_0) = \mathcal{T} \exp \left[-i \int_{t_0}^t dt_1 \hat{\Xi}_F(t_1) \right]. \quad (\text{B15})$$

$\mathcal{T}$ is the time ordering. This provides a means for developing a perturbation expansion in the perturbing potential $\hat{\Xi}(t)$ starting from a Floquet system. Although we have focused on a time-periodic $\hat{H}_0(t)$, the derivation makes no assumption of a time-periodic Hamiltonian.

APPENDIX C: FERMI GOLDEN RULE IN FLOQUET SYSTEMS

The Fermi golden rule in Floquet systems is also derived in Secs. 2.1 and 2.3 of Ref. [3] and the Supplemental Material of Ref. [19].

To first order in the perturbing field

$$|\Psi_F(t)\rangle = \left[1 - i \int_{t_0}^t dt_1 \hat{\Xi}_F(t_1) \right] |\Psi_F(t_0)\rangle. \quad (\text{C1})$$

Returning to the Schrödinger picture, one finds

$$|\Psi(t)\rangle = \hat{U}_0(t, t_0) \left[1 - i \int_{t_0}^t dt_1 \hat{\Xi}_F(t_1) \right] |\Psi_F(t_0)\rangle. \quad (\text{C2})$$

With an initial state $|\Psi_F(t_0)\rangle = |\Phi_{\alpha}(t_0)\rangle$, the transition amplitude to a final state $|\Phi_{\beta}(t)\rangle$, with $\beta \neq \alpha$, is given by

$$\begin{aligned} \langle\Phi_{\beta}(t)|\Psi(t)\rangle &= -i \int_{t_0}^t dt_1 \langle\Phi_{\beta}(t)|\hat{U}_0(t, t_1)\hat{\Xi}(t_1)|\Phi_{\alpha}(t_1)\rangle \\ &\quad \times e^{-iE_{\alpha}(t_1-t_0)} \\ &= -i \int_{t_0}^t dt_1 \langle\Phi_{\beta}(t_1)|\hat{\Xi}(t_1)|\Phi_{\alpha}(t_1)\rangle \\ &\quad \times e^{-iE_{\beta}(t-t_1)} e^{-iE_{\alpha}(t_1-t_0)}, \end{aligned} \quad (\text{C3})$$

where Eq. (B6) has been utilized. The transition probability is given by

$$\begin{aligned} &|\langle\Phi_{\beta}(t)|\Psi(t)\rangle|^2 \\ &= \left| \int_{t_0}^t dt_1 \langle\Phi_{\beta}(t_1)|\hat{\Xi}(t_1)|\Phi_{\alpha}(t_1)\rangle e^{i(E_{\beta}-E_{\alpha})t_1} \right|^2. \end{aligned} \quad (\text{C4})$$

For a harmonic perturbation with an arbitrary frequency ω

$$\hat{\Xi}(t) = \hat{\Xi} e^{i\omega t} + \hat{\Xi}^{\dagger} e^{-i\omega t}. \quad (\text{C5})$$

Let

$$a = \int_{t_0}^t dt_1 \langle\Phi_{\beta}(t_1)|\hat{\Xi}|\Phi_{\alpha}(t_1)\rangle e^{i(\omega+\Delta_{\beta\alpha})t_1}, \quad (\text{C6})$$

$$b = \int_{t_0}^t dt_1 \langle\Phi_{\beta}(t_1)|\hat{\Xi}^{\dagger}|\Phi_{\alpha}(t_1)\rangle e^{i(-\omega+\Delta_{\beta\alpha})t_1}, \quad (\text{C7})$$

where $\Delta_{\beta\alpha} = E_{\beta} - E_{\alpha}$. Since the Floquet modes are periodic in time, one may write the matrix elements as Fourier series:

$$\langle\Phi_{\beta}(t_1)|\hat{\Xi}|\Phi_{\alpha}(t_1)\rangle = \sum_n f_n^{\beta\alpha} e^{in\Omega t_1}, \quad (\text{C8})$$

$$\langle\Phi_{\beta}(t_1)|\hat{\Xi}^{\dagger}|\Phi_{\alpha}(t_1)\rangle = \sum_n f_n^{\alpha\beta*} e^{-in\Omega t_1}. \quad (\text{C9})$$

One obtains

$$a = \sum_n f_n^{\beta\alpha} \int_{t_0}^t dt_1 e^{i(\omega+n\Omega+\Delta_{\beta\alpha})t_1}, \quad (\text{C10})$$

$$b = \sum_n f_n^{\alpha\beta*} \int_{t_0}^t dt_1 e^{i(-\omega+n\Omega+\Delta_{\beta\alpha})t_1}. \quad (\text{C11})$$

Assuming that $t_0 = 0$ one finds

$$\begin{aligned} a &= \sum_n f_n^{\beta\alpha} \frac{e^{i(\omega+n\Omega+\Delta_{\beta\alpha})t} - 1}{i(\omega+n\Omega+\Delta_{\beta\alpha})} \\ &= \sum_n f_n^{\beta\alpha} e^{i(\omega+n\Omega+\Delta_{\beta\alpha})t/2} \frac{2 \sin[(\omega+n\Omega+\Delta_{\beta\alpha})t/2]}{\omega+n\Omega+\Delta_{\beta\alpha}}, \end{aligned} \quad (\text{C12})$$

$$\begin{aligned} b &= \sum_n f_n^{\alpha\beta*} \frac{e^{i(-\omega+n\Omega+\Delta_{\beta\alpha})t} - 1}{i(-\omega+n\Omega+\Delta_{\beta\alpha})} \\ &= \sum_n f_n^{\alpha\beta*} e^{i(-\omega+n\Omega+\Delta_{\beta\alpha})t/2} \frac{2 \sin[(\omega-n\Omega-\Delta_{\beta\alpha})t/2]}{\omega-n\Omega-\Delta_{\beta\alpha}}. \end{aligned} \quad (\text{C13})$$

The absolute value squared of the transition amplitude is

$$|\langle \Phi_\beta(t) | \Psi(t) \rangle|^2 = |a+b|^2 = |a|^2 + |b|^2 + a^*b + ab^*. \quad (\text{C14})$$

In the limit $t \rightarrow \infty$,

$$\begin{aligned} |a|^2 &= 4 \sum_n |f_n^{\beta\alpha}|^2 \frac{\sin^2[(\omega+n\Omega+\Delta_{\beta\alpha})t/2]}{(\omega+n\Omega+\Delta_{\beta\alpha})^2} \\ &= 2\pi t \sum_n |f_n^{\beta\alpha}|^2 \delta(\omega+n\Omega+\Delta_{\beta\alpha}), \end{aligned} \quad (\text{C15})$$

$$\begin{aligned} |b|^2 &= 4 \sum_m |f_m^{\alpha\beta}|^2 \frac{\sin^2[(\omega-m\Omega-\Delta_{\beta\alpha})t/2]}{(\omega-m\Omega-\Delta_{\beta\alpha})^2}, \\ &= 2\pi t \sum_m |f_m^{\alpha\beta}|^2 \delta(\omega-m\Omega-\Delta_{\beta\alpha}). \end{aligned} \quad (\text{C16})$$

If $2\Delta_{\beta\alpha}/\Omega = M$ (integer), then the cross terms can contribute when $n = -m - 2M$:

$$\begin{aligned} a^*b + ab^* &= 4\pi t \sum_m \text{Re}[f_m^{\alpha\beta} f_{-m-2M}^{\beta\alpha}] \delta(\omega-m\Omega-\Delta_{\beta\alpha}). \end{aligned} \quad (\text{C17})$$

Equations (C15), (C16), and (C17) represent umklapp in frequency space for absorption and emission processes associated to Floquet system.

APPENDIX D: TRAVELING WAVE POTENTIAL: BAND SPLITTING

For the traveling wave potential, the Floquet-Schrödinger equation, Eq. (21), is the matrix equation for $c_{\omega,k}$, where the matrix formally involves infinitely many (ω, k) points. As in the textbook example of band splitting, the infinite matrix reduces to a two-by-two matrix when one is close to the Floquet-Brillouin zone edge induced by the potential, so that only two zones are relevant. The relevant 2×2 matrix is

$$\begin{pmatrix} \frac{k^2}{2m_e} + m\Omega & \frac{V_0}{2} \\ \frac{V_0}{2} & \frac{(k-\kappa)^2}{2m_e} + (m+1)\Omega \end{pmatrix} = \begin{pmatrix} E_0(k, m) & \frac{1}{2}V_0 \\ \frac{1}{2}V_0 & E_0(k-\kappa, m+1) \end{pmatrix},$$

where $E_0(k, m) = \frac{k^2}{2m_e} + m\Omega$ are the matrix elements without the potential present. The eigenvalues of this matrix are

$$\begin{aligned} 2\lambda_{\pm} &= E_0(k, m) + E_0(k-\kappa, m+1) \\ &\pm \sqrt{(E_0(k, m) - E_0(k-\kappa, m+1))^2 + V_0^2}. \end{aligned} \quad (\text{D1})$$

Thus, the effect of the applied potential is largest when $E_0(k, m) = E_0(k-\kappa, m+1)$, i.e., when $k^2/2m_e = (k-\kappa)^2/2m_e + \Omega$, so $k = \kappa/2 + m_e\Omega/\kappa$. For the time-independent situation, $\Omega = 0$, this reduces to the usual condition $k = \kappa/2$, so that splitting is maximal at the edge of the new Bloch Brillouin zone induced by the potential. For the time-dependent case, the point of strongest coupling shifts away from the Brillouin zone edge, and $m_e\Omega/\kappa$ gives the relevant scale. Note that our potential is a traveling wave, which breaks symmetries and leads to a difference between $+k$ and $-k$.

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