The Time Dependent Variational Principle and Semi-Classical Dynamics

J. M. B. Lopes dos Santos

Department of Physics and Astronomy,

Faculdade de Ciências da Universidade do Porto,

*and CFUM/CFP, Universidade do Minho e Universidade do Porto**

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Abstract

The derivation of semi-classical dynamics of electrons in bands, in weak and slowly varying fields is notoriously tricky. The existence of the anomalous Hall effect ultimately revealed the need to consider the effects of the Berry curvature of the band in the semi classical equations of motion. The modern framework to include such effects has been provided by the work of [1] who resort to a variational principle to derive the equations of motion of the parameters defining a wave packet. We review their method as applied to a set of tight-binding bands.

* jlsantos@fc.up.pt

I. SCHRÖDINGER EQUATION FROM VARIATIONAL PRINCIPLE

The time dependent variational principle can be traced apparently to Dirac, but the classic reference is the work of [2]. The basic principle is to define an action for a arbitrary evolution in Hilbert space and derive the Schrödinger time dependent equation as an extremum of this action. The proposed action for a Hamiltonian $\hat{H}$ is

$$S = \int dt \mathcal{L}(\overline{\psi}, \psi) = \int dt \langle \psi(t) | \, i\hbar \frac{d}{dt} - \hat{H} \, | \psi(t) \rangle \tag{1}$$

The trajectories we vary in this Lagrangian are arbitrary paths $|\psi(t)\rangle$ in the Hilbert space of the system. The present form of the Lagrangian requires that $|\psi(t)\rangle$ is always normalized. The method can formulated without this restriction [Kramer and Saraceno [2]].

Let us proceed. The principle states the action is stationary for a true evolution of the system:

$$\delta S = \int dt \delta \mathcal{L}(\overline{\psi}, \psi) = 0 \tag{2}$$

Now,

$$\begin{aligned} \delta \mathcal{L}(\overline{\psi}, \psi) &= i\hbar \left[\langle \psi | \delta \dot{\psi} \rangle + \langle \delta \psi | \dot{\psi} \rangle \right] - \langle \delta \psi | \, \hat{H} \, | \psi \rangle - \langle \psi | \, \hat{H} \, | \delta \psi \rangle \\ &= i\hbar \left[\frac{d}{dt} \langle \psi | \delta \psi \rangle + \langle \delta \psi | \dot{\psi} \rangle - \langle \dot{\psi} | \delta \psi \rangle \right] - \langle \delta \psi | \, \hat{H} \, | \psi \rangle - \langle \psi | \, \hat{H} \, | \delta \psi \rangle \end{aligned} \tag{3}$$

We can ignore the full time derivative (it integrates to zero) and get

$$\begin{aligned} \delta S = & \int dt \, \langle \delta \psi | \left[i\hbar \frac{d}{dt} | \psi \rangle - H | \psi \rangle \right] \\ & + \int dt \left[-i\hbar \frac{d}{dt} \langle \psi | - \langle \psi | \, \hat{H} \right] | \delta \psi \rangle = 0 \end{aligned} \tag{4}$$

Sufficient conditions for an extremum are

$$i\hbar \frac{d}{dt} | \psi \rangle - \hat{H} | \psi \rangle = 0 \tag{5}$$

$$-i\hbar \frac{d}{dt} \langle \psi | - \langle \psi | \, \hat{H} = 0 \tag{6}$$

which are the known equations of motion.

II. PARAMETRIZING THE TRAJECTORY

A. Free particle in 1D

To apply this as a variational principle to obtain wave packet dynamics, we parametrize the state $|\psi(t)\rangle$ with semi-classical coordinates and the require the action to have an extremum in these restricted trajectories. We illustrate with the case of a free particle in one dimension (1D).

Take $|\psi(t)\rangle$ to be a 1D wave packet parametrized by a center $x_c(t)$ and a momentum $p_c(t)$:

$$|\psi_c(t)\rangle = \int \frac{dp}{2\pi}\varphi\left(p; p_c(t), x_c(t)\right)|p\rangle \tag{7}$$

To lighten the notation, we use $\varphi\left(p; p_c(t), x_c(t)\right) \to \varphi_c(p)$. We can insure the state is normalized at all times with

$$\int \frac{dp}{2\pi}\left|\varphi_c(p)\right|^2 = 1 \tag{8}$$

The function $\varphi_c(p)$ is peaked about p_c with

$$\langle\psi_c(t)|\,\hat{p}\,|\psi_c(t)\rangle = \int \frac{dp}{2\pi}p\left|\varphi(p)\right|^2 = p_c \tag{9}$$

The wave packet is also localized at x_c

$$\langle\psi_c(t)|\,\hat{x}\,|\psi_c(t)\rangle = \int \frac{dp}{2\pi}\varphi_c^*\left(p\right)\left(i\hbar\frac{\partial}{\partial p}\right)\varphi_c\left(p\right) = x_c \tag{10}$$

We assume that the momentum and position are well defined and express this fact by assuming that for any slowly varying function of x or p

$$\int \frac{dp}{2\pi}f(x,p)\left|\varphi_c(p)\right|^2 \approx f(x_c, p_c) \tag{11}$$

If we write

$$\varphi_c\left(p\right) = e^{-i\gamma_c(p)}\left|\varphi_c\left(p\right)\right|, \tag{12}$$

is is easy to see that the equation for x_c is (the position operator in the p-representation is $\hat{x} = i\hbar\partial/dp$)

$$x_c = \hbar\int \frac{dp}{2\pi}\left|\varphi_c\left(p\right)\right|^2\frac{\partial\gamma_c}{\partial p} \approx \hbar\left.\frac{\partial\gamma_c(p)}{\partial p}\right|_{p=p_c} \tag{13}$$

The term involving the derivative of $|\varphi(p)|$ is zero because of the normalization condition. In summary, we may set $\gamma = (p/\hbar)\,x_c$ and our wave-packet (WP) is

$$|\psi_c(t)\rangle = \int \frac{dp}{2\pi}e^{-i(p/\hbar)x_c}\left|\varphi_c\left(p\right)\right||p\rangle \tag{14}$$

We now derive the equations of motion for $x_c(t), p_c(t)$ by requiring the action to be stationary. Note, that we are not deriving the true evolution of the system because we are forcing the shape of $|\psi(t)\rangle$, only allowing for variation of $x_c(t)$ and $p_c(t)$.

Our Lagrangian is (do not confuse: in this context , p_c is a generalized coordinate not a momentum)

$$\mathcal{L}\left(x_c, p_c; \dot{x}_c, \dot{p}_c\right) = \langle\psi_c(t)|\, i\hbar\frac{d}{dt} - \hat{H}\, |\psi_c(t)\rangle \tag{15}$$

We denote

$$\langle\psi_c(t)|\, \hat{H}\, |\psi_c(t)\rangle := \mathcal{H}\left(x_c, p_c\right) \tag{16}$$

and

$$i\hbar\frac{d}{dt}\, |\psi_c(t)\rangle = i\hbar\left(\dot{x}_c\, |\partial_{x_c}\psi_c\rangle + \dot{p}_c\, |\partial_{p_c}\psi_c\rangle\right) \tag{17}$$

because the only variation allowed in the WP is that of the coordinates x_c and p_c.

Therefore, the Lagrangian is

$$\begin{aligned}\mathcal{L}\left(x_c, p_c; \dot{x}_c, \dot{p}_c\right) &= i\hbar\left[\dot{x}_c X(x_c, p_c) + \dot{p}_c P(x_c, p_c)\right] - \mathcal{H}(x_c, p_c) &(18)\\ &= i\hbar\left[\dot{x}_c X_c + \dot{p}_c P_c\right] - \mathcal{H}_c &(19)\end{aligned}$$

with

$$\begin{aligned}X_c &:= \langle\psi_c|\partial_{x_c}\psi_c\rangle &(20)\\ P_c &:= \langle\psi_c|\partial_{p_c}\psi_c\rangle &(21)\end{aligned}$$

We could calculate immediately X_c and P_c as functions of x_c, p_c using Eq. (14) but, for the moment, we keep them unspecified. Consistent with our notation we indicate their dependence on (x_c,p_c) our generalized coordinates by a subscript,

We vary the Lagrangian with respects to the coordinates x_c, p_c as

$$\delta\mathcal{L} = i\hbar\left[\delta\dot{x}_c X_c + \dot{x}_c\delta X_c + \delta\dot{p}_c P_c + \dot{p}_c\delta P_c\right] - \delta\mathcal{H}_c = 0 \tag{22}$$

We integrate by parts the variation of the action $\delta S = \delta S = \int dt\delta\mathcal{L}$ and throw away full derivatives, as they are without consequence in the equations of motion

$$i\hbar\left[-\delta x_c\dot{X}_c + \dot{x}_c\delta X_c - \delta p_c\dot{P}_c + \dot{p}_c\delta P_c(x_c, p_c)\right] - \delta\mathcal{H}(x_c, p_c) = 0 \tag{23}$$

We now use

$$\dot{X}_c = \dot{x}_c \frac{\partial X_c}{\partial x_c} + \dot{p}_c \frac{\partial X_c}{\partial p_c} \tag{24}$$

$$\dot{P}_c = \dot{x}_c \frac{\partial P_c}{\partial x_c} + \dot{p}_c \frac{\partial P_c}{\partial p_c} \tag{25}$$

and

$$\delta X_c = \frac{\partial X_c}{\partial x_c}\delta x_c + \frac{\partial X_c}{\partial p_c}\delta p_c \tag{26}$$

$$\delta P_c = \frac{\partial P_c}{\partial x_c}\delta x_c + \frac{\partial P_c}{\partial p_c}\delta p_c \tag{27}$$

Gathering terms,

$$\int dt \delta \mathcal{L} = i\hbar \int dt \left[\delta x_c \left(-\dot{x}_c \frac{\partial X_c}{\partial x_c} - \dot{p}_c \frac{\partial X_c}{\partial p_c} + \dot{x}_c \frac{\partial X_c}{\partial x_c} + \dot{p}_c \frac{\partial P_c}{\partial x_c} - \frac{1}{i\hbar}\frac{\partial \mathcal{H}_c}{\partial x_c} \right) \right. \tag{28}$$

$$\left. + \delta p_c \left(-\dot{p}_c \frac{\partial P_c}{\partial p_c} - \dot{x}_c \frac{\partial P_c}{\partial x_c} + \dot{p}_c \frac{\partial P_c}{\partial p_c} + \dot{x}_c \frac{\partial X_c}{\partial p_c} - \frac{1}{i\hbar}\frac{\partial \mathcal{H}_c}{\partial p_c} \right) \right] = 0 \tag{29}$$

Because the variations are independent

$$-i\hbar \dot{p}_c \left(\frac{\partial X_c}{\partial p_c} - \frac{\partial P_c}{\partial x_c} \right) = \frac{\partial \mathcal{H}}{\partial x_c} \tag{30}$$

$$-i\hbar \dot{x}_c \left(\frac{\partial P_c}{\partial x_c} - \frac{\partial X_c}{\partial p_c} \right) = \frac{\partial \mathcal{H}}{\partial p_c} \tag{31}$$

For our WP, Eq. (14)

$$X_c = \left[\int \frac{dp}{2\pi} \left(-ip/\hbar\right) \left|\varphi_c(p)\right|^2 \right] = -ip_c/\hbar \tag{32}$$

$$P = \int \frac{dp}{2\pi} e^{i(p/\hbar)x_c} \left|\varphi_c(p)\right| \frac{\partial}{\partial p_c} e^{-i(p/\hbar)x_c} \left|\varphi_c(p)\right|$$

$$= \frac{1}{2}\frac{\partial}{\partial p_c} \int \frac{dp}{2\pi} \left|\varphi(p)\right|^2 = 0 \tag{33}$$

and

$$\frac{\partial X_c}{\partial p_c} = -\frac{i}{\hbar} \tag{34}$$

$$\frac{\partial P_c}{\partial x_c} = 0 \tag{35}$$

The equations of motion reduce to

$$\dot{p}_c = -\frac{\partial \mathcal{H}}{\partial x_c} \tag{36}$$

$$\dot{x}_c = \frac{\partial \mathcal{H}}{\partial p_c} \tag{37}$$

and the Lagrangian is simply

$$\dot{x}_c p_c - \mathcal{H}(x_c, p_c) \tag{38}$$

This is exactly as expected for a free particle.

B. Free Particle in external Field

A slightly more involved case in that a particle moving in an electromagnetic field:

$$H = \frac{\hbar^2}{2m}\left[-i\nabla_{\mathbf{r}} - \frac{q}{\hbar}\mathbf{A}(\mathbf{r},t)\right]^2 + q\phi(\mathbf{r}) \tag{39}$$

We can define our plane wave

$$\langle \mathbf{r}|\mathbf{p}\rangle = e^{i\mathbf{p}\cdot\mathbf{r}} \tag{40}$$

Suppose we have a WP centered about $\mathbf{r}_c(t)$ in real space

$$|\psi_c(t)\rangle = \int \frac{d^3\mathbf{p}}{(2\pi)^3} w_c(\mathbf{p})\,|\mathbf{p}\rangle \tag{41}$$

The normalization condition is $\left(\langle \mathbf{p}|\mathbf{p}'\rangle = (2\pi)^3\,\delta\left(\mathbf{p}-\mathbf{p}'\right)\right)$

$$\int \frac{d^3\mathbf{p}}{(2\pi)^3}\,|w_c(\mathbf{p})|^2 = 1 \tag{42}$$

For this particular Hamiltonian (as for the later case of a band) it proves useful to do a change of variable,$\mathbf{p}\to\mathbf{k}$, $\hbar\mathbf{k} = \mathbf{p} - q\mathbf{A}(\mathbf{r}_c,t)$, and write

$$|\psi_c(t)\rangle = \int \frac{d^3\mathbf{k}}{(2\pi)^3} w_c(\mathbf{k})\,|\hbar\mathbf{k} + q\mathbf{A}(\mathbf{r}_c,t)\rangle \tag{43}$$

The position operator is still

$$\mathbf{r} = i\hbar\nabla_{\mathbf{p}} = i\nabla_{\mathbf{k}} \tag{44}$$

and so

$$\begin{aligned}\langle\psi_c|\,\mathbf{r}_c\,|\psi_c\rangle &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} w_c^*(\mathbf{k}) i\nabla_{\mathbf{k}} w_c(\mathbf{k}) \\ & \int \frac{d^3\mathbf{k}}{(2\pi)^3}\left(\nabla_{\mathbf{k}}\gamma_{\mathbf{k}}\right)|w_c(\mathbf{k})|^2 = \mathbf{r}_c\end{aligned} \tag{45}$$

This means that our previous choice of $\gamma_{\mathbf{k}} = \mathbf{k}\cdot\mathbf{r}_c$ still gives a WP centered in real space about $\mathbf{r}_c$. Our WP is

$$|\psi_c(t)\rangle = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\,|w_c(\mathbf{k})|\,e^{-i\mathbf{k}\cdot\mathbf{r}_c}\,|\hbar\mathbf{k} + q\mathbf{A}(\mathbf{r}_c,t)\rangle \tag{46}$$

Since

$$\langle \mathbf{r}|\hbar\mathbf{k}+q\mathbf{A}(\mathbf{r}_c,t)\rangle = e^{i(\mathbf{k}+q\mathbf{A}(\mathbf{r}_c,t))\cdot\mathbf{r}}, \tag{47}$$

in real space the WP looks like

$$\begin{aligned}\psi_c(\mathbf{r},t) = \langle \mathbf{r}|\psi_c(t)\rangle &= \int \frac{d^3\mathbf{k}}{(2\pi)^3}\,|w_c(\mathbf{k})|\, e^{-i\mathbf{k}\cdot\mathbf{r}_c} e^{i[\mathbf{k}+q\mathbf{A}(\mathbf{r}_c,t)]\cdot\mathbf{r}} \\ &= e^{i(q/\hbar)\mathbf{A}(\mathbf{r}_c,t)\cdot\mathbf{r}} \int \frac{d^3\mathbf{k}}{(2\pi)^3}\,|w_c(\mathbf{k})|\, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r_c}]}\end{aligned} \tag{48}$$

All we did with the change of variable was add a phase factor $\exp\left[i\,(q/\hbar)\,\mathbf{A}(\mathbf{r}_c,t)\cdot\mathbf{r}\right]$ to the wave function. This is still a linear superposition of plane waves (the shift in wave vector $\mathbf{k}\to\mathbf{k}+(q/\hbar)\,\mathbf{A}(\mathbf{r}_c,t)$ is independent of $\mathbf{r}$) but, at fixed $\mathbf{k}$, the plane wave of amplitude $|w_c(\mathbf{k})|$ has different wave vectors at different times,namely

$$\mathbf{q}(t) = \mathbf{k} + (q/\hbar)\,\mathbf{A}\left(\mathbf{r}_c(t),t\right)$$

We are now using $\mathbf{k}_c$ and $\mathbf{r}_c$ as parameters of the WP. This change of variable is well known in classical physics. There are two momenta in the presence of a vector potential: $\mathbf{p}$ is the canonical momentum, conjugate to $\mathbf{r}$; but the $m\mathbf{v}$ momentum in *not* $\mathbf{p}$, it is $m\mathbf{v}=\mathbf{p}-q\mathbf{A}$, in our case $\hbar\mathbf{k}$, as we shall soon find out.

There is an interesting consequence of our choice of coordinates in the mean energy; since

$$\left[-i\hbar\nabla - q\mathbf{A}(\mathbf{r},t)\right]|\mathbf{k}+q\mathbf{A}(\mathbf{r}_c,t)\rangle = \hbar\mathbf{k} - q\left(\mathbf{A}(\mathbf{r},t)-\mathbf{A}(\mathbf{r}_c,t)\right)|\hbar\mathbf{k}+q\mathbf{A}(\mathbf{r}_c)\rangle \tag{49}$$

we get

$$\begin{aligned}\langle\psi_c|\,\hat{H}\,|\psi_c\rangle &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} w^*(\mathbf{k}) \left[\frac{1}{2m}\left(\hbar\mathbf{k} - q\left(\mathbf{A}(\mathbf{r},t)-\mathbf{A}(\mathbf{r}_c,t)\right)\right)^2 + q\phi(\mathbf{r})\right] w^*(\mathbf{k}) \\ &= \frac{\hbar^2\mathbf{k}_c^2}{2m} + q\phi(\mathbf{r}_c)\end{aligned} \tag{50}$$

where we used Eq. (11) to make the vector potential disappear from the classical Hamiltonian. It has been gauged away by the phase factor added to the wave-function.

The Lagrangian still has the general form

$$\mathcal{L}(\mathbf{r}_c,\mathbf{k}_c,\dot{\mathbf{r}}_c,\dot{\mathbf{k}}_c) = \langle\psi_c(t)|\, i\hbar\frac{d}{dt} - \hat{H}\,|\psi_c(t)\rangle\,, \tag{51}$$

but now there is an extra factor in the time derivative of $|\psi_c(t)\rangle$ coming from $\mathbf{A}(\mathbf{r}_c,t)$

$$\langle\psi_c(t)|\, i\hbar\frac{d}{dt}\,|\psi_c(t)\rangle = i\hbar\left(-i\mathbf{k}\cdot\dot{\mathbf{r}}_c + i\frac{q}{\hbar}\dot{\mathbf{A}}(\mathbf{r}_c,t)\cdot\mathbf{r}_c\right) \tag{52}$$

because, once again

$$\begin{aligned}\mathbf{P}_c = \langle\psi_c|\nabla_{\mathbf{k}_c}\psi_c\rangle &= \int \frac{d^3\mathbf{k}}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}_c} w_c^*(\mathbf{k}) \nabla_{\mathbf{k}_c} e^{i\mathbf{k}\cdot\mathbf{r}_c} w_c(\mathbf{k}) \\ &= \frac{1}{2}\nabla_{\mathbf{k}_c} \int \frac{d^3\mathbf{k}}{(2\pi)^3} |w_c(\mathbf{k})|^2 = 0 \end{aligned} \tag{53}$$

Therefore

$$\mathcal{L}(\mathbf{r}_c, \mathbf{k}_c; \dot{\mathbf{r}}_c, \dot{\mathbf{k}}_c) = \dot{\mathbf{r}}_c \cdot \hbar\mathbf{k}_c - q\dot{\mathbf{A}}(\mathbf{r}_c, t)\cdot\mathbf{r}_c - \left(\frac{\hbar^2\mathbf{k}_c^2}{2m} + q\phi(\mathbf{r}_c)\right) \tag{54}$$

Let us now derive the Euler-Lagrange equations of motion. The terms proportional do $\delta\mathbf{k}_c$ are

$$\left(\dot{\mathbf{r}}_c - \frac{\hbar\mathbf{k}_c}{m}\right)\cdot\delta\mathbf{k}_c \tag{55}$$

To obtain the term is $\delta\mathbf{r}_c$ requires more work; we will not worry about total derivatives;

$$\begin{aligned}\delta\dot{\mathbf{r}}_c\cdot\hbar\mathbf{k}_c &= -\hbar\dot{\mathbf{k}}_c\cdot\delta\mathbf{r}_c + \frac{d}{dt}(\dots) \\ \delta\left[q\dot{\mathbf{A}}(\mathbf{r}_c,t)\cdot\mathbf{r}_c\right] &= q\dot{\mathbf{A}}(\mathbf{r}_c,t)\cdot\delta\mathbf{r}_c - q\delta\mathbf{A}\cdot\dot{\mathbf{r}}_c + \frac{d}{dt}(\dots) \\ &= q\frac{\partial\mathbf{A}}{\partial t}\cdot\delta\mathbf{r}_c - q\left[\frac{\partial A^\beta}{\partial r_c^\alpha}\dot{r}_c^\alpha\delta r_c^\beta - \frac{\partial A^\beta}{\partial r_c^\alpha}\dot{r}_c^\beta\delta r_c^\alpha\right] \\ &= q\frac{\partial\mathbf{A}}{\partial t}\cdot\delta\mathbf{r}_c - q\left(\frac{\partial A^\beta}{\partial r^\alpha}\dot{r}^\alpha\delta r^\beta - \frac{\partial A^\alpha}{\partial r^\beta}\dot{r}^\alpha\delta r^\beta\right) \\ &= q\frac{\partial\mathbf{A}}{\partial t}\cdot\delta\mathbf{r}_c + q\left(\frac{\partial A^\alpha}{\partial r^\beta} - \frac{\partial A^\beta}{\partial r^\alpha}\right)\dot{r}^\alpha\delta r^\beta \end{aligned} \tag{56}$$

$$\delta\left[q\phi(\mathbf{r}_c)\right] = q\nabla\phi\cdot\delta\mathbf{r}_c \tag{57}$$

The equations of motion become

$$\dot{\mathbf{r}}_c = \frac{\hbar\mathbf{k}_c}{m} \tag{58}$$

$$\hbar\dot{k^\beta}_c = q\left[-\frac{\partial\phi}{\partial r_c^\beta} - \frac{\partial A^\beta}{\partial t}\right] + q\mathcal{F}^{\beta\alpha}\dot{r}^\alpha \tag{59}$$

with

$$\mathcal{F}^{\beta\alpha} := \frac{\partial A^\alpha}{\partial r^\beta} - \frac{\partial A^\beta}{\partial r^\alpha} \tag{60}$$

in 3D

$$B^\gamma = \frac{1}{2}\epsilon^{\gamma\beta\alpha}\mathcal{F}^{\beta\alpha} = \frac{1}{2}\epsilon^{\gamma\beta\alpha}\left(\frac{\partial A^\alpha}{\partial r^\beta} - \frac{\partial A^\beta}{\partial r^\alpha}\right) = \epsilon^{\gamma\beta\alpha}\frac{\partial A^\alpha}{\partial r^\beta} = (\nabla\times\mathbf{A})^\gamma \tag{61}$$

and

$$
\begin{aligned}
(\dot{\mathbf{r}}\times\mathbf{B})^{\beta} &= \epsilon^{\beta\alpha\gamma}\dot{r}^{\alpha}B^{\gamma} = \frac{1}{2}\epsilon^{\beta\alpha\gamma}\epsilon^{\gamma\mu\nu}\dot{r}^{\alpha}\mathcal{F}^{\mu\nu} = \frac{1}{2}\left(\delta_{\beta\mu}\delta_{\alpha\nu}-\delta_{\beta\nu}\delta_{\alpha\mu}\right)\dot{r}^{\alpha}\mathcal{F}^{\mu\nu} \\
&= \mathcal{F}^{\beta\alpha}\dot{r}^{\alpha} \qquad (62)
\end{aligned}
$$

or

$$\dot{\mathbf{r}}_c = \frac{\hbar\mathbf{k}_c}{m} \qquad (63)$$

$$\hbar\dot{\mathbf{k}}_c = q\left[\mathbf{E}+\dot{\mathbf{r}}_c\times\mathbf{B}\right] \qquad (64)$$

These are the expected classical equations of motion. The second term in the Lorentz force. As stated above, $\hbar\mathbf{k}$ is the $m\mathbf{v}$ momentum, and so the second equation is Newton's second law for a particle in the presence of electric and magnetig fields.

III. THE EQUATIONS OF MOTION IN BANDS

A. Wave Packet of Bloch States

The only adaptation we need to do from the free electron example to a band is to consider a superposition of Bloch states of a single band

$$|\psi_c(t)\rangle = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} w_c(\mathbf{k})\,|\psi_{\mathbf{k}s}\rangle \qquad (65)$$

As before, $|w_c(\mathbf{k})|^2$,is peaked about $\mathbf{k}_c$ and normalized in the large V limit:

$$\int\frac{d^3k}{(2\pi)^3}\,|w_c(\mathbf{k})|^2 = 1, \qquad (66)$$

$$\int\frac{d^3k}{(2\pi)^3}\mathbf{k}\,|w_c(\mathbf{k})|^2 = \mathbf{k}_c, \qquad (67)$$

The state is also peaked about $\mathbf{r}_c$ in real space.

$$\langle\psi_c(t)|\,\hat{\mathbf{r}}\,|\psi_c(t)\rangle = \mathbf{r}_c \qquad (68)$$

For slowly varying functions of $\mathbf{k}$ and $\mathbf{r}$

$$\int\frac{d^3k}{(2\pi)^3}f\left(\hat{\mathbf{r}},\mathbf{k}\right)|w_c(\mathbf{k})|^2 \approx f\left(\mathbf{r}_c,\mathbf{k}_c\right), \qquad (69)$$

To proceed we need the position operator in the $\mathbf{k}$ representation;

$$\hat{\mathbf{r}} \rightarrow i\nabla_{\mathbf{k}} + \boldsymbol{\xi}_{\mathbf{k}ss} \tag{70}$$

where the Berry connection, $\boldsymbol{\xi}_{\mathbf{k},s's}$ is defined by

$$\boldsymbol{\xi}_{\mathbf{k},s's} := \frac{i}{v_c}\int_{uc} d^d r u^*_{\mathbf{k}s'}\left(\mathbf{r}\right)\nabla_{\mathbf{k}} u_{\mathbf{k}s}\left(\mathbf{r}\right), \tag{71}$$

$u_{\mathbf{k}s}\left(\mathbf{r}\right)$ is the periodic component of the Bloch wave function of band s and v_c the volume of the unit cell. The chosen normalization is

$$\langle u_{\mathbf{k}s}|u_{\mathbf{k}s'}\rangle_{uc} := \frac{1}{v_c}\int_{uc} d^d r u^*_{\mathbf{k}s}\left(\mathbf{r}\right) u_{\mathbf{k}s'}(\mathbf{r}) = \delta_{ss'} \tag{72}$$

From here on, since we are working only with one band, we drop the band index s. Continuing

$$\langle\psi_c(t)|\,\hat{\mathbf{r}}\,|\psi_c(t)\rangle = \int \frac{d^3k}{(2\pi)^3} w_c(\mathbf{k})\left(i\nabla_{\mathbf{k}} + \boldsymbol{\xi}_{\mathbf{k}}\right) w_c(\mathbf{k}) \tag{73}$$

If, as before,

$$w_c(\mathbf{k}) = |w_c(\mathbf{k}))|\, e^{-i\gamma_c(\mathbf{k})} \tag{74}$$

we get

$$\begin{aligned}\langle\psi_c(t)|\,\hat{\mathbf{r}}\,|\psi_c(t)\rangle &= \int \frac{d^3k}{(2\pi)^3}\left(\nabla_{\mathbf{k}}\gamma(\mathbf{k}) + \boldsymbol{\xi}_{\mathbf{k}}\right)|w_c(\mathbf{k})|^2 = \mathbf{r}_c \\ &= \nabla_{\mathbf{k}}\gamma_c(\mathbf{k})|_{\mathbf{k}=\mathbf{k}_c} + \boldsymbol{\xi}_{\mathbf{k}_c} = \mathbf{r}_c \end{aligned} \tag{75}$$

We choose

$$\gamma_c(\mathbf{k}) := \mathbf{k}\cdot\mathbf{r}_c - (\mathbf{k}-\mathbf{k}_c)\cdot\boldsymbol{\xi}_{\mathbf{k}} \tag{76}$$

Then

$$\nabla_{\mathbf{k}}\gamma_c(\mathbf{k})|_{\mathbf{k_c}} = \mathbf{r}_c - \boldsymbol{\xi}_{\mathbf{k}_c}. \tag{77}$$

and

$$\langle\psi(t)|\mathbf{r}\,|\psi(t)\rangle = \int \frac{d^3k}{(2\pi)^3}\left(\nabla_{\mathbf{k}}\gamma(\mathbf{k}) + \boldsymbol{\xi}_{\mathbf{k}}\right)|w_c(\mathbf{k})|^2 = \nabla_{\mathbf{k}}\gamma_c(\mathbf{k})|_{\mathbf{k_c}} + \boldsymbol{\xi}_{\mathbf{k}_c} \tag{78}$$

$$= \mathbf{r}_c \tag{79}$$

where we used Eq. (69).With this choice

$$\mathbf{X} := \langle \psi_c(t) | \nabla_{\mathbf{r}_c} \psi_c(t) \rangle = -i\mathbf{k} \tag{80}$$

$$\mathbf{P} = \langle \psi_c(t) | \nabla_{\mathbf{k}_c} \psi_c(t) \rangle = -i\boldsymbol{\xi}_{\mathbf{k}_c} \tag{81}$$

and the Lagrangian density is

$$\mathcal{L} = \dot{\mathbf{r}}_c \cdot \hbar\mathbf{k}_c - \hbar\dot{\mathbf{k}}_c \cdot \boldsymbol{\xi}_{\mathbf{k}_c} - \mathcal{H}(\mathbf{k}_c, \mathbf{r}_c) \tag{82}$$

In the case of an unperturbed band we can simply write

$$\mathcal{H}(\mathbf{k}_c, \mathbf{r}_c) = \epsilon(\mathbf{k}_c) \tag{83}$$

From this point on, we will refer only to the WP coordinates, and can, without confusion with the Bloch vector of position operator, drop the c index. The beauty of this treatment is that we already considered a Lagrangian of this form

$$\mathcal{L} = \dot{\mathbf{r}} \cdot \hbar\mathbf{k} - \hbar\dot{\mathbf{k}} \cdot \boldsymbol{\xi}_{\mathbf{k}} - \epsilon(\mathbf{k}) \tag{84}$$

Up to a total derivative it has the form

$$\mathcal{L} = \dot{\mathbf{r}} \cdot \hbar\mathbf{k} + \dot{\boldsymbol{\xi}}_{\mathbf{k}} \cdot \hbar\mathbf{k} - \epsilon(\mathbf{k})$$

If we compare it to Eq. (54), we see that $\boldsymbol{\xi}_{\mathbf{k}}$ is equivalent to the term $-q\mathbf{A}$,except that it works as a vector potential *momentum space.* The equations of motion become simply

$$\begin{aligned} \hbar\dot{\mathbf{k}} &= 0 \\ \dot{\mathbf{r}} &= \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon(\mathbf{k}) - \dot{\mathbf{k}}\times\boldsymbol{\omega}(\mathbf{k}) \end{aligned}$$

with

$$\boldsymbol{\omega}(\mathbf{k}) := \nabla_{\mathbf{k}} \times \boldsymbol{\xi}_{\mathbf{k}}$$

called the Berry curvature. Just like the vector potential changes the phase of the WP as is moves through real space, the Berry connection $\boldsymbol{\xi}_{\mathbf{k}}$ expresses a change of phase (Berry Phase) as the state moves in the Brillouin zone. The Berry curvature amounts to a "magnetic" field in Bloch space. In the absence of external fields though, there is no effect of this term, since $\hbar\dot{\mathbf{k}} = 0$.

B. Perturbed Bands

We now arrive at the problem we are really interested in: what happens when we perturb the bands with an external field?

The Hamiltonian is now

$$\hat{H} = \frac{1}{2m}\left(-i\hbar\nabla_{\mathbf{r}} - q\mathbf{A}(\mathbf{r})\right)^2 + V_L(\mathbf{r}) + q\phi(\mathbf{r},t) \tag{85}$$

where $V_L(\mathbf{r})$ is the lattice potential. We build our wave packet,as before, using Bloch states

$$|\psi_c(t)\rangle = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} w_c(\mathbf{k})\,|\psi_{\mathbf{k}s}\rangle \tag{86}$$

where

$$\langle\mathbf{r}|\psi_{\mathbf{k}}\rangle = \frac{1}{\sqrt{V}} e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}s}(\mathbf{r}) \tag{87}$$

We can repeat the same gauge transformations and define

$$\langle\mathbf{r}|\widetilde{\psi}_{\mathbf{k}}\rangle = \frac{1}{\sqrt{V}} e^{i[\mathbf{k}+(q/\hbar)\mathbf{A}(\mathbf{r}_c)]\cdot\mathbf{r}} u_{\mathbf{k}s}(\mathbf{r}) \tag{88}$$

Note that the "magnetic Bloch states" $\left|\widetilde{\psi}_{\mathbf{k}}\right\rangle$ are still orthogonal for different $\mathbf{k}'s$ and remain normalized.

$$|\psi_c(t)\rangle = \frac{1}{\sqrt{V}}\sum_{\mathbf{k}} w_c(\mathbf{k})\left|\widetilde{\psi}_{\mathbf{k}s}\right\rangle \tag{89}$$

Within approximations that we have been doing,

$$\begin{aligned}\langle\psi_c(t)|\,\hat{H}\,|\psi_c(t)\rangle &\approx \langle\psi_c(t)|\,\frac{1}{2m}\left(-i\hbar\nabla_{\mathbf{r}}\right)^2 + V_L(\mathbf{r}) + q\phi(\mathbf{r}_c,t)\,|\psi_c(t)\rangle \\ &\approx \epsilon(\mathbf{k}_c) + q\phi(\mathbf{r}_c,t)\end{aligned} \tag{90}$$

where $\epsilon(\mathbf{k}_c)$ in the unperturbed band energy. To ensure the WP is peaked about $\mathbf{r}_c$, we again choose $w(\mathbf{k}) = |w(\mathbf{k})|\exp(-i\gamma_{\mathbf{k}})$ with

$$\gamma_c(\mathbf{k}) := \mathbf{k}\cdot\mathbf{r}_c - (\mathbf{k}-\mathbf{k}_c)\cdot\boldsymbol{\xi}_{\mathbf{k}} \tag{91}$$

When we compute the Lagrangian, as in the case of the free particle, we must include in the term

$$\langle\psi_c(t)|\,\frac{d}{dt}\,|\psi_c(t)\rangle \tag{92}$$

the term coming from the time derivative of $\exp\left[i(q/\hbar)\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}\right]$. So the full Lagrangian becomes

$$\mathcal{L} = \dot{\mathbf{r}}_c \cdot \hbar\mathbf{k}_c - \hbar\dot{\mathbf{k}}_c \cdot \boldsymbol{\xi}_{\mathbf{k}_c} - q\dot{\mathbf{A}}(\mathbf{r}_c, t)\cdot\mathbf{r}_c - \left[\epsilon(\mathbf{k}_c) + q\phi(\mathbf{r}_c, t)\right] \tag{93}$$

Our previous analysis then leads to the semi-classical equations of motion of electrons in a band

$$\dot{\mathbf{r}} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon(\mathbf{k}) - \dot{\mathbf{k}} \times \omega\left(\mathbf{k}\right) \tag{94}$$

$$\hbar\dot{\mathbf{k}} = q\left(\mathbf{E} + \dot{\mathbf{r}} \times \mathbf{B}\right) \tag{95}$$

IV. TRANSPORT IN MAGNETIC BLOCH BANDS

There is an interesting generalization of these results in [3]. In the presence of a uniform magnetic field $\mathbf{B}_0$ that satisfies a commensurability condition (flux ϕ per unit cell is a rational fraction of the of the flux quantum h/e, $\phi/\phi_0 = p/q$) one can still apply Bloch's theorem with a larger unit cell that contains q of the original cells of the crystal. What Chang and Niu consider in [3] is the motion of electrons in the magnetic Bloch bands under the presence of an electric field and an *extra* magnetic field $\delta\mathbf{B}$ (which may not be uniform or may drive the total field from the commensurability condition. I will not give the details of this generalization but only mention that the semi-classical equations of motion are almost unchanged

$$\dot{\mathbf{r}} = \frac{1}{\hbar}\nabla_{\mathbf{k}}E(\mathbf{k}) - \dot{\mathbf{k}} \times \omega\left(\mathbf{k}\right) \tag{96}$$

$$\hbar\dot{\mathbf{k}} = -e\left(\mathbf{E} + \dot{\mathbf{r}} \times \delta\mathbf{B}\right) \tag{97}$$

I say *almost* because the band energy $E\left(\mathbf{k}\right)$ is modified by the extra magnetic field as

$$E(\mathbf{k}) = \epsilon(\mathbf{k}) + \frac{e}{2m}\delta\mathbf{B}\cdot\mathbf{L}$$

where $\mathbf{L}$ is the angular momentum of the wave-packet

$$\mathbf{L} := \langle W|\left(\mathbf{r} - \mathbf{r}_c\right) \times \left(-i\hbar\nabla_{\mathbf{r}}\right)|W\rangle$$

If $\delta\mathbf{B} = 0$, we obtain the same equations of motion as before without the *uniform* field $\mathbf{B}_0$. But remember the dispersion $\epsilon(\mathbf{k})$ refers to the magnetic Bloch bands.

Appendix A: Classical equations of motion in a magnetic field

The classical Hamiltonian for a charge q in an electromagnetic field is

$$H(\mathbf{r},\mathbf{p}) = \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A}(\mathbf{r},t)\right) + q\phi(\mathbf{r}) \tag{A1}$$

The Hamilton equations become

$$\dot{\mathbf{r}} = \frac{1}{m}\left(\mathbf{p} - q\mathbf{A}(\mathbf{r},t)\right) \tag{A2}$$

$$\dot{p}_i = \frac{q}{m}\left(p_j - qA_j(\mathbf{r},t)\right)\frac{\partial}{\partial x_i}A_j(\mathbf{r},t) - q\frac{\partial}{\partial x_i}\phi \tag{A3}$$

These look quite different from the known Newton's law with the Lorentz force. In fact they are not, but we require the distinction between the canonical momentum $\mathbf{p}$ and the $m\mathbf{v} :=\mathbf{k}$ momentum of Newtonian physics. Note first that

$$\mathbf{v} = \dot{\mathbf{r}} = \frac{1}{m}\left(\mathbf{p} - q\mathbf{A}(\mathbf{r},t)\right) = \frac{\mathbf{k}}{m} \tag{A4}$$

and

$$\dot{p}_i = qv_j\frac{\partial}{\partial x_i}A_j(\mathbf{r},t) - q\frac{\partial}{\partial x_i}\phi \tag{A5}$$

We resort to the identity

$$\begin{aligned}
\left[\mathbf{v}\times(\nabla\times\mathbf{A})\right]_i &= \epsilon_{ijk}\epsilon_{klm}v_j\partial_l A_m \\
&= \epsilon_{kij}\epsilon_{klm}v_j\partial_l A_m \\
&= \left(\delta_{il}\delta_{jm} - \delta_{im}\delta_{jl}\right)v_j\partial_l A_m In \\
&= v_j\partial_i A_j - v_j\partial_j A_i
\end{aligned} \tag{A6}$$

other words

$$v_j\partial_i A_j = \left[\mathbf{v}\times(\nabla\times\mathbf{A})\right]_i + (\mathbf{v}\cdot\nabla)A_i \tag{A7}$$

and the second Hamilton equation is

$$\dot{\mathbf{p}} - q(\mathbf{v}\cdot\nabla)A_i = q\mathbf{v}\times(\nabla\times\mathbf{A}) - q\frac{\partial}{\partial x_i}\phi \tag{A8}$$

Now note that

$$\dot{\mathbf{k}} = \dot{\mathbf{p}} - q\dot{\mathbf{A}}(\mathbf{r},t) = \dot{\mathbf{p}} - q\frac{\partial\mathbf{A}}{\partial t} - q(\dot{\mathbf{r}}\cdot\nabla)\mathbf{A} \tag{A9}$$

so

$$\dot{\mathbf{k}} = q\mathbf{v}\times\mathbf{B} + q\left(-\frac{\partial\mathbf{A}}{\partial t} - \frac{\partial}{\partial x_i}\phi(\mathbf{r})\right) \tag{A10}$$

or

$$\mathbf{v} = \frac{\mathbf{k}}{m} \tag{A11}$$

$$\dot{\mathbf{k}} = q\left(\mathbf{E} + \mathbf{v} \times \mathbf{B}\right) \tag{A12}$$

The Lorentz force is the time derivative of $\mathbf{k}$, the $m\mathbf{v}$ momentum, not of $\mathbf{p}$, the canonical momentum. In semi-classical equations of motion in a band the Bloch momentum $\hbar\mathbf{k}$ is the canonical momentum, so we expect the semi-classical equations of motion to be expressed in the $\hbar\mathbf{q} := \hbar\mathbf{k} - q\mathbf{A}$.

Appendix B: How does the wave packet move

In this we start with our WP and apply directly the evolution operator without resorting to the time dependent variational method. The aim is to show that the dynamics arises from the terms in the Hamiltonian linear in the deviations $\mathbf{r} - \mathbf{r}_c$ and $\mathbf{k} - \mathbf{k}_c$.

$$|\psi_c(t)\rangle = \int \frac{d^3\mathbf{k}}{(2\pi)^3} |w_c(\mathbf{k})| \, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r_c}]} \, |\hbar\mathbf{k} + q\mathbf{A}(\mathbf{r}_c)\rangle \tag{B1}$$

with wave function

$$\psi_c(\mathbf{r}, t) = e^{i(q/\hbar)\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}} \int \frac{d^3\mathbf{k}}{(2\pi)^3} |w_c(\mathbf{k})| \, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r_c}]} \tag{B2}$$

The question is whether we can understand the motion of the parameters $\mathbf{r}_c$ and $\mathbf{k}_c$ when we apply directly the evolution operator to this wave-packet. Recall that $|w_c(\mathbf{k})|$ is peaked about $\mathbf{k}_c$ and the wave packet is localized in real space about r_c

$$\left[-i\hbar\nabla - q\mathbf{A}(\mathbf{r}, t)\right] |\mathbf{k} + q\mathbf{A}(\mathbf{r}_c)\rangle = \hbar\mathbf{k} - q\left(\mathbf{A}(\mathbf{r}, t) - \mathbf{A}(\mathbf{r}_c, t)\right) |\hbar\mathbf{k} + q\mathbf{A}(\mathbf{r}_c)\rangle \tag{B3}$$

$$e^{-i\hat{H}t/\hbar} |\mathbf{k} + q\mathbf{A}(\mathbf{r}_c)\rangle = \exp\left[i\left(\frac{\hbar}{2m}\left[\mathbf{k} - \frac{q}{\hbar}\left(\mathbf{A}(\hat{\mathbf{r}}, t) - \mathbf{A}(\mathbf{r}_c, t)\right)\right]^2 + qV(\hat{\mathbf{r}})\right) t\right] |\mathbf{k} + q\mathbf{A}(\mathbf{r}_c)\rangle \tag{B4}$$

Now we use the fact that we may assume that $\mathbf{k} \approx \mathbf{k}_c$ and after integration over $\mathbf{k}$, $\mathbf{r} \approx \mathbf{r}_c$. So we expand these expressions to linear order in the deviations. We can drop constant factors independent of $\mathbf{k}$ and $\mathbf{r}$ as these only change the phase of the wave function and do not affect either $\mathbf{r}_c$ or $\mathbf{k}_c$

$$qV(\hat{\mathbf{r}}) \to -q\mathbf{E}(\mathbf{r}_c)\cdot(\hat{\mathbf{r}}-\mathbf{r}_c) \tag{B5}$$

$$\left[\mathbf{k}-\frac{q}{\hbar}\left(\mathbf{A}(\hat{\mathbf{r}},t)-\mathbf{A}(\mathbf{r}_c,t)\right)\right]^2 \to \left[\mathbf{k}_c+(\mathbf{k}-\mathbf{k}_c)-\frac{q}{\hbar}\left(\left[(\mathbf{r}-\mathbf{r}_c)\cdot\nabla_{\mathbf{r}_c}\right]\mathbf{A}(\mathbf{r}_c,t)\right)\right]^2 \tag{B6}$$

Ignoring terms which do not depend on $\mathbf{k}$ or $\mathbf{r}$ this becomes

$$2\left[\mathbf{k}\cdot\mathbf{k}_c-\frac{q}{\hbar}\left[(\mathbf{r}-\mathbf{r}_c)\cdot\nabla_{\mathbf{r}_c}\right]\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{k}_c\right] \tag{B7}$$

We now need to transform the term

$$\frac{q}{\hbar}\left[(\hat{\mathbf{r}}-\mathbf{r}_c)\cdot\nabla_{\mathbf{r}_c}\right]\mathbf{A}(\mathbf{r}_c)\cdot\frac{\hbar\mathbf{k}_c}{m}t=\frac{q}{\hbar}\left(r^\alpha-r_c^\alpha\right)\frac{\partial}{\partial r^\alpha}A^\beta(r_c)\frac{\hbar k_c^\beta}{m}t; \tag{B8}$$

we note that

$$\begin{aligned}[\mathbf{v}\times(\nabla\times\mathbf{A})]^\alpha &= \epsilon^{\alpha\beta\gamma}v^\beta\epsilon^{\gamma\mu\nu}\partial_\mu A^\nu\\ &=\delta_{\alpha\mu}\delta_{\beta\nu}v^\beta\partial_\mu A^\nu-\delta_{\alpha\nu}\delta_{\beta\mu}v^\beta\partial_\mu A^\alpha\\ &=\partial_\alpha(\mathbf{v}\cdot\mathbf{A})-(\mathbf{v}\cdot\nabla)\,A^\alpha\end{aligned} \tag{B9}$$

which, in our problem translates to

$$\frac{q}{\hbar}\left[(\hat{\mathbf{r}}-\mathbf{r}_c)\cdot\nabla_{\mathbf{r}_c}\right]\mathbf{A}(\mathbf{r}_c)\cdot\frac{\hbar\mathbf{k}_c}{m}t=\frac{q}{\hbar}(\hat{\mathbf{r}}-\mathbf{r}_c)\cdot\left[\frac{\hbar\mathbf{k}_c}{m}t\times(\nabla\times\mathbf{A})\right]+\frac{q}{\hbar}(\hat{\mathbf{r}}-\mathbf{r}_c)^\alpha\left(\frac{\hbar\mathbf{k}_c}{m}t\cdot\nabla\right)A^\alpha(\mathbf{r}_c) \tag{B10}$$

which we rewrite as (consistently with keeping linear terms in the deviation from $\mathbf{k}_c$ and $\mathbf{r}_c$

$$\frac{q}{\hbar}(\hat{\mathbf{r}}-\mathbf{r}_c)\cdot\left[\frac{\hbar\mathbf{k}_c}{m}t\times(\nabla\times\mathbf{A})\right]+\frac{q}{\hbar}(\hat{\mathbf{r}}-\mathbf{r}_c)^\alpha\left[A^\alpha(\mathbf{r}_c+\hbar\mathbf{k}_c t/m)-A^\alpha(\mathbf{r}_c)\right] \tag{B11}$$

Dropping again constant phases we arrive at

$$\begin{aligned}&\exp\left[-i\left(\frac{\hbar}{2m}\left[\mathbf{k}-\frac{q}{\hbar}\left(\mathbf{A}(\hat{\mathbf{r}},t)-\mathbf{A}(\mathbf{r}_c,t)\right)\right]^2+qV(\hat{\mathbf{r}})\right)t\right]\to\\ &\exp -i\left[\mathbf{k}\cdot\frac{\hbar\mathbf{k}_c}{m}t-\frac{q}{\hbar}\left[(\hat{\mathbf{r}}-\mathbf{r}_c)\cdot\left(\mathbf{E}t+\frac{\hbar\mathbf{k}_c}{m}t\times(\nabla\times\mathbf{A})\right)\right]-\frac{q}{\hbar}\hat{\mathbf{r}}\cdot\left(A^\alpha(\mathbf{r}_c+\hbar\mathbf{k}_c t/m)-A^\alpha(\mathbf{r}_c)\right)\right]\end{aligned} \tag{B12}$$

Now we can read the changes of WP parameters. The term in $\mathbf{k}$ modifies $\mathbf{r}_c$. The terms in $\mathbf{r}-\mathbf{r}_c$ shift $\mathbf{k}_c$ and the last term modifies the phase factor

$$\mathbf{r}_c \to \mathbf{r}_c+\frac{\hbar\mathbf{k}_c}{m}t \tag{B13}$$

$$\mathbf{k}_c \to \mathbf{k}_c+\frac{q}{\hbar}\left(\mathbf{E}+\frac{\hbar\mathbf{k}_c}{m}\times(\nabla\times\mathbf{A})\right)t \tag{B14}$$

and the last term is what is required to change the phase factor to

$$e^{i(q/\hbar)\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}} \rightarrow e^{i(q/\hbar)\mathbf{A}(\mathbf{r}_c+\hbar\mathbf{k}_c t/m)\cdot\mathbf{r}} = e^{i(q/\hbar)\mathbf{A}(\mathbf{r}_c(t))\cdot\mathbf{r}} \tag{B15}$$

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