LECTURES ON SUPERCONDUCTIVITY

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LECTURE 2
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EFFECTS OF THE VECTOR POTENTIAL IN QUANTUM MECHANICS

Reminder: the vector potential $\boldsymbol{A}(\boldsymbol{r},t)$ in classical mechanics

The classical equation of motion of a charged particle in an electric field $\boldsymbol{E}$ and magnetic field $\boldsymbol{B}$:

$$m\frac{d\mathbf{V}}{dt} = e(\boldsymbol{E} + \mathbf{v} \times \boldsymbol{B}) + \mathbf{F}_{\text{non-em}}$$

where $\mathbf{F}_{\text{non-em}}$ are any forces of non-electromagnetic origin. But for many purposes (e.g. stat. mech.) need to express this in terms of Hamiltonian formalism:

How to find $H(\boldsymbol{r},\boldsymbol{p})$ s.t.

$$\frac{d\boldsymbol{r}}{dt} = \frac{\partial H}{\partial \boldsymbol{p}}\ , \qquad \frac{d\boldsymbol{p}}{dt} = -\frac{\partial H}{\partial \boldsymbol{r}} \qquad ?$$

Solution: define $\boldsymbol{A}(\boldsymbol{r},t)$ s.t.

$$\boldsymbol{E}(\boldsymbol{r},t) = -\nabla\Phi(\boldsymbol{r}t) - \frac{\partial \boldsymbol{A}(\boldsymbol{r},t)}{\partial \boldsymbol{t}}\ , \qquad \boldsymbol{B}(\boldsymbol{r},t) = \boldsymbol{\nabla} \times \boldsymbol{A}(\boldsymbol{r},t)$$

where $\Phi(rt)$ is the static Coulomb potential

(hence $\boldsymbol{\nabla} \times \boldsymbol{E} = -\partial\mathbf{B}/\partial$t)

↑ Faraday

and put

$$H(\boldsymbol{r},\boldsymbol{p}) = \left(\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r},t)\right)^2/2m + e\Phi(\boldsymbol{r}t) + V_{non-em}$$

This works! (see Appendix)

note: $\mathbf{v} \equiv \frac{d\boldsymbol{r}}{dt} = \frac{\partial H}{\partial \boldsymbol{p}} = \frac{1}{\boldsymbol{m}}\left(\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r},t)\right) \qquad (\neq \boldsymbol{p}/m)$

so first term in $H(\boldsymbol{r},\boldsymbol{p}) = \frac{1}{2}m\mathrm{v}^2$ = kinetic energy (only)!

(but expressed in terms of **p** and $\boldsymbol{A}$).

Quantum mechanics:

$\boldsymbol{p} \rightarrow -\boldsymbol{i\hbar\nabla}$ so KE is

$$\widehat{\boldsymbol{H}}_{\boldsymbol{K}} = (-i\hbar\boldsymbol{\nabla} - e\boldsymbol{A})^{\mathbf{2}}/2m$$

and so, including possible $\mathrm{V}_{non-em} + e\Phi(\boldsymbol{r}t) \equiv \mathrm{V}(\boldsymbol{r}t)$,

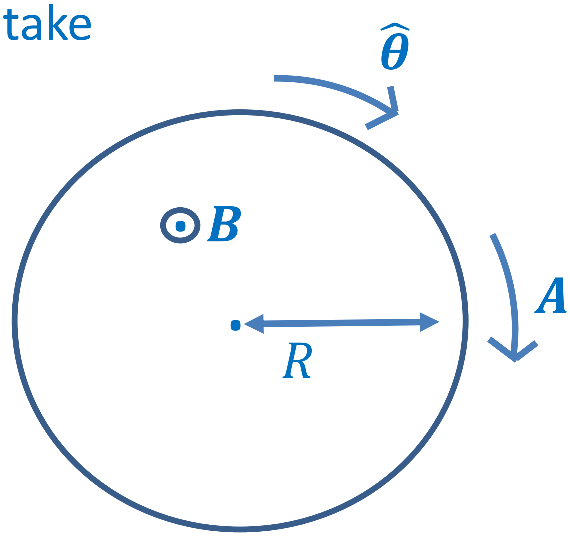
$$\widehat{H} = \frac{1}{2m}\left(-i\hbar\boldsymbol{\nabla} - e\boldsymbol{A}(rt)\right)^2 + \mathrm{V}(\boldsymbol{r}t)$$

In CM (classical mechanics), all effects obtainable from $\boldsymbol{A}(\boldsymbol{r},t)$ are equally derivable only from $\boldsymbol{E}(\boldsymbol{r},t)$ and $\boldsymbol{B}(\boldsymbol{r},t)$ ⇒ vector potential redundant. In QM (quantum mechanics) this is not true: $\boldsymbol{A}(\boldsymbol{r},t)$ has a "life of its own"!

Single charged particle on thin ring

If field $\boldsymbol{B}$ through ring is uniform, can take

$$\boldsymbol{A} \equiv A_\theta \hat{\boldsymbol{\theta}} \ , A_\theta \equiv \frac{1}{2} BR$$



then flux Φ through ring is

$$\Phi \equiv \pi R^2 B \Rightarrow A_\theta = \Phi/2\pi R$$

TISE for $\psi \equiv \psi(\theta)$ is

$$\hat{H}\psi(\theta) \equiv \frac{1}{2m}\big(-i\hbar\boldsymbol{\nabla} - e\boldsymbol{A}(\boldsymbol{r})\big)^2 \psi(\theta) = E\psi(\theta)$$

only nonzero component of $\boldsymbol{\nabla}$ is $\boldsymbol{\nabla}_{\boldsymbol{\theta}} = \frac{1}{R}\frac{\partial}{\partial\theta}$

and only component of $\boldsymbol{A}$ is A_θ, so

$$\frac{\hbar^2}{2mR^2}\left(-i\frac{\partial}{\partial\theta} - \frac{e}{\hbar}A_\theta R\right)^2 \psi(\theta) = E\psi(\theta)$$

or putting $A_\theta = \Phi/2\pi R$ and defining $\Phi_o^{sp} \equiv h/e$

(single-particle) flux quantum

$$\frac{\hbar^2}{2mR^2}\left(-i\frac{\partial}{\partial\theta} - \Phi/\Phi_o^{sp}\right)^2 \psi(\theta) = E\psi(\theta)$$

$= \hat{L}_z$ (angular momentum in units of $\hbar$)

Formal solution is

$$\psi(\theta) = \exp ik\theta \ , (k \text{ arbitrary}), \quad E = \frac{\hbar^2}{2mR^2}\left(k - \Phi/\Phi_o^{Sp}\right)^2$$

However, crucial point:

$\psi(\theta)$ must be single-valued, i.e. $\psi(\theta + 2n\pi) = \psi(\theta)$ (SVBC)

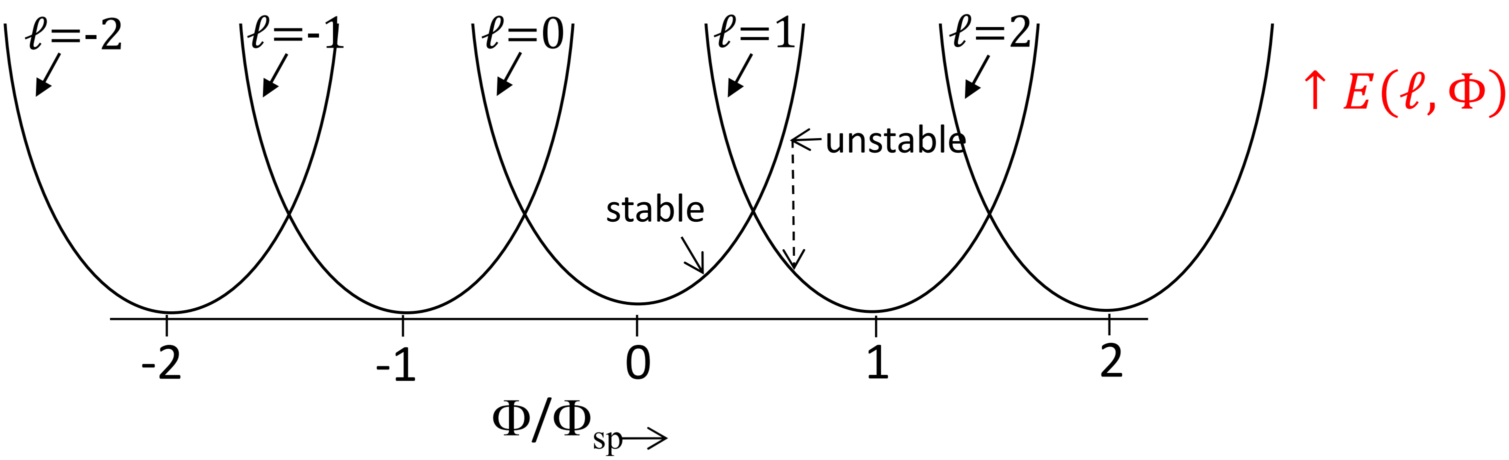
single-valuedness boundary condition

Hence, only allowed values of k are integers $\ell = 0, \pm 1, \pm 2$ ...

(i.e. angular momentum $\hat{L}_z$ is quantized in units of $\hbar$)

Thus,

$$\psi_\ell(\theta) = \exp i\ell\theta \ , \ \ell = 0, \pm 1, \pm 2 \ ,$$



$$j_\ell(\Phi) = \frac{e\hbar}{mR}\left(\ell - \Phi/\Phi_o^{sp}\right) = \text{slope of curve}$$

For $\Phi < \Phi_o^{sp}/2$,

GS has $\ell = 0 \Rightarrow p_\theta \equiv L_z/R = \ell\hbar/R = 0$

However, recall that in the presence of $\boldsymbol{A}$, $\mathbf{v} \neq \boldsymbol{p}/m$! In fact,

$$\mathbf{v} = (\boldsymbol{p} - e\boldsymbol{A})/m \Rightarrow \mathbf{v}_\theta = -eA_\theta/m$$

$\Rightarrow \mathbf{j}_\theta \equiv e\mathrm{v}_\theta = -(e^2/m)A_o \neq 0$ in general, in sense to produce magnetic field opposite to $\boldsymbol{B} \Rightarrow$ GS is diamagnetic,

$$\mathbf{j}_\theta = -(e^2/m)A_\theta \neq 0$$

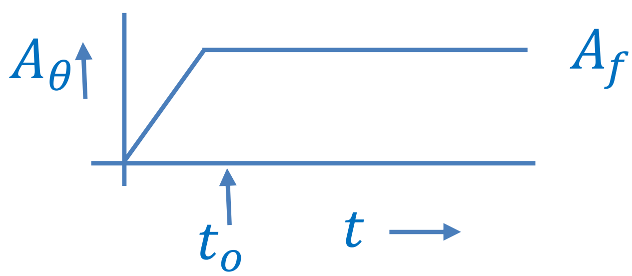
Single charged particle on ring: two notes

1. What is the situation in classical mechanics?

We can still formally introduce $\ell \equiv L_z/\hbar$ and write

$$E(\ell) = \frac{\hbar^2}{2mR^2}\left(\ell - \Phi/\Phi_o^{Sp}\right)^2$$

but now there is no restriction on ℓ (SVBC is meaningless since no wave function!) so now GS always corresponds to $\ell = \Phi/\Phi_o^{sp}$, equivalent to $\mathbf{j}_\theta = 0$ (no diamagnetism).



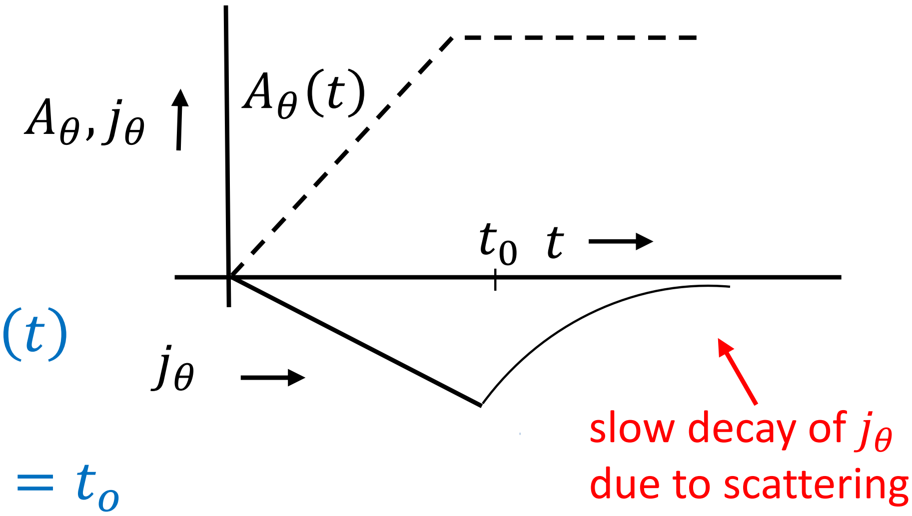
However, consider time-dependent problem: since motion is restricted to ring, Lorenz force $\mathbf{v} \times \boldsymbol{B}$ is irrelevant and we have by Newton II

$$m\frac{d\mathbf{v}}{dt} = e\boldsymbol{E}(t) = -e\frac{\partial \boldsymbol{A}}{\partial t}$$

or

$$m\frac{d\mathrm{v}_\theta}{dt} = -e\frac{dA_\theta}{dt}$$

If at $t = 0$ $\quad v_\theta = 0$, solution is simply

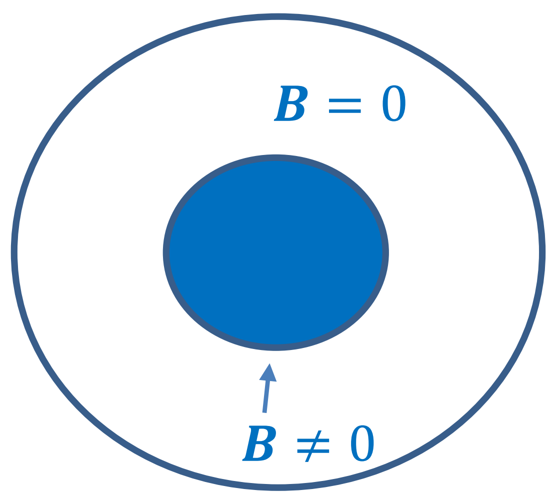


$$v_\theta(t) = -(e/m)A_\theta(t)$$

and in particular for $t = t_o$
$v_\theta = -(e/m)A_f \Rightarrow j_\theta = -(e^2/m)A_f$
as in Quantum Mechanics case. However, this is not the lowest-energy state, so scattering by walls, etc. will reduce j_θ to zero.

2. Aharonov-Bohm effect

note induced diamagnetic current depends only on total trapped flux Φ, not on details of how it is produced. Hence in particular can get nonzero effect even when $\boldsymbol{B} = 0$ everywhere on ring! (e.g. $\boldsymbol{B}$ produced by "Helmholtz coil")



Atomic diamagnetism

To the extent that argument applies, velocity of electrons at radius r given by

$$\boldsymbol{v}(\boldsymbol{r}) = -e\boldsymbol{A}(\boldsymbol{r})/m$$

but electric current density $\boldsymbol{j}(\boldsymbol{r}) = n(\boldsymbol{r})e\boldsymbol{v}(\boldsymbol{r})$, hence

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{-n(r)e^2}{m}\boldsymbol{A}(\boldsymbol{r})$$

Circulating current produces magnetic field ΔB opposite to the original one. $\Rightarrow$ diamagnetism.

Estimate order of magnitude of ΔB at nucleus: ignoring factors of 2π, etc., $A \sim BR_{at}$,

$J \sim R_{at}^2 j \sim -R_{at}^2 ne^2 A/m$, or since $nR_{at}^3 \sim Z$ (no. of electrons in atom)

$\sim(-Ze^2/mR_{at})A \sim -(Ze^2/m)B$,

and by Biot-Savart $\Delta B \sim \dfrac{\mu_o J}{R_{at}} \sim -\left(\dfrac{Ze^2\mu_o}{mR_{at}}\right)B$:

$(Ze^2\mu_o/mR_{at}) \sim 10^{-2}$

(actually, with all the geometrical factors, close to 10^{-5}) so $\Delta B/B \ll 1$ (but must still be taken into account for accurate NMR work

Superconductors: London phenomenology

Basic postulate: as in atomic diamagnetism,

$$\boldsymbol{j}(\boldsymbol{r}) = \frac{-ne^2}{m}\boldsymbol{A}(\boldsymbol{r})$$

Combine with Maxwell's equation

$$\boldsymbol{j} = \boldsymbol{\nabla} \times \boldsymbol{H} \equiv \frac{1}{\mu_o}\boldsymbol{\nabla} \times \boldsymbol{B} = \frac{1}{\mu_o}\boldsymbol{\nabla} \times (\boldsymbol{\nabla} \times \boldsymbol{A}) = -\frac{1}{\mu_o}\nabla^2 \boldsymbol{A}$$

(div $\boldsymbol{A} = 0$)

gives

$$\nabla^2 \boldsymbol{A} = +\frac{ne^2}{m}\mu_O \boldsymbol{A}$$

or taking curl.

$$\nabla^2 \boldsymbol{B} = \frac{ne^2\mu_O}{m}\boldsymbol{B} \equiv \lambda_L^{-2}\boldsymbol{B}$$

London penetration depth

Hence, both in atomic diamagnets and in superconductors,

$$B \sim B_o \exp - \mathrm{z}/\lambda_L$$

($\mathrm{n}(r)$, hence λ_L, comparable in two cases)

Qualitative difference: in both cases $\lambda_L \sim 10^{-5}$cm, but:

in atomic diamagnets, $\lambda_L \gg$ atomic size $\Rightarrow$ effect very small

in superconductors, $\lambda_L \ll$ size of sample $\Rightarrow$ effect spectacular: magnetic field totally excluded from bulk (Meissner effect)

Problems with London phenomenology

A. Meissner effect is thermodynamically stable phenomenon, circulating supercurrents are (usually) metastable. Hence London argument does not explain stability of supercurrents! (↑: beware misleading statements in literature)

B. No explanation of vanishing Peltier coefficient.

C. Why do not all metals show Meissner effect?

Let's turn question C around: when does Meissner effect not occur?

1. Classical systems:

no restriction on $v_\theta \equiv (p_\theta - eA_\theta)/m$, and by Maxwellian statistical mechanics $P(v_\theta) \propto \exp(-\frac{1}{2}mv_\theta^2/kT)$, hence from symmetry $\bar{v}_\theta = 0 \Rightarrow$ no circulating current $\Rightarrow$ no diamagnetism (Bohr-van Leeuwen theorem)

2. Quantum Mechanics, but noninteracting particles obeying classical statistics: now p (or angular momentum L) is quantized

$$L = \ell\hbar\,, \qquad \ell = \;\ldots -2, -1, 0, 1, 2\ldots$$

and energy $\propto \left(\ell - \Phi/\Phi_o^{sp}\right)^2 \hbar^2/2mR^2 \quad \Phi_o^{sp} \equiv h/e$

so

$$P(\ell) \propto \exp -\left\{\left(\ell - \Phi/\Phi_o^{sp}\right)^2 \cdot \hbar^2/2mR^2 k_B T\right\} \quad \left(\Phi \lesssim \Phi_o^{sp}\right)$$

Crucial point: under normal circumstances $k_B T \gg \hbar^2/2mR^2$, so can effectively replace discrete values of ℓ by continuum $\Rightarrow$ back to classical mechanics.*

3. So, will only get Meissner effect if for some reason all or most particles forced to be in same state. Then the probability of angular momentum ℓ for this state is

$$P(\ell) \propto \exp\, - N_o(\ell - \Phi/\Phi_o)^2\, \hbar^2/2\mathrm{m}R^2 k_B T$$

↑ Number of particles in same state

and provided $k_B T$, though $\gg \hbar^2/2mR^2$, is $\ll N\hbar^2/2mR^2$, can get results similar to atomic diamagnetism.

Does this ever happen? Yes, e.g. for noninteracting gas of bosons!

*Doesn't work for atomic diamagnetism because $\hbar^2/2mR^2$ is $\sim eV$, hence $\gg k_B T$.

electron volts ↗

Summary of lecture 2:

(1) In presence of electromagnetic vector potential $\boldsymbol{A}(\boldsymbol{r})$, Hamiltonian for single particle of charge e is

$$\hat{H} = \left(\frac{-i\hbar\boldsymbol{\nabla}}{2m} - e\boldsymbol{A}(\boldsymbol{r})\right)^2 + V(r)$$

(2) For single particle on ring, in flux $\Phi < \frac{1}{2}h/e$, this leads in ground state to $j_\theta = -(e^2/m)A_\theta$

(3) For a closed-shell atom, similar argument leads to

$$\boldsymbol{j}(\boldsymbol{r}) = -\frac{n(r)e^2}{m}\boldsymbol{A}(\boldsymbol{r})$$ (diamagnetism) (*)

(4) London phenomenology: assume (*) also describes superconductor

$\Rightarrow$ Meissner effect

(5) Difficulty: doesn't work for classical systems (Bohr – van Leeuwen theorem) nor (for $kT \gtrsim \hbar^2/mR^2$) for quantum systems obeying Maxwell-Boltzmann statistics

(6) Difficulty can be overcome if for some reason all particles forced to behave in same way.

Appendix Derivation of the classical equations of motion from the Hamiltonian written in terms of the vector potential.

We consider the classical Hamiltonian of a particle of charge e in a specified magnetic vector potential $\boldsymbol{A}(\boldsymbol{r}t)$:

$$H(\boldsymbol{r},\boldsymbol{p}:t) \equiv \frac{1}{2m}\left(\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r}t)\right)^2 + e\Phi(rt) + \mathrm{V}_{non-em}(\boldsymbol{r}t) \qquad (1)$$

where $\boldsymbol{A}(\boldsymbol{r}t)$ satisfies the conditions (consistent with Faraday's law)

$$\boldsymbol{B}(\boldsymbol{r}t) = \boldsymbol{\nabla} \times \boldsymbol{A}(\boldsymbol{r}t), \quad \boldsymbol{E}(\boldsymbol{r}t) = -\boldsymbol{\nabla}\Phi(rt) - \frac{\partial \boldsymbol{A}(\boldsymbol{r}t)}{\partial t} \qquad (2a,b)$$

We wish to show that the Hamiltonian equations

$$\frac{d\boldsymbol{r}}{dt} = \frac{\partial H}{\partial \boldsymbol{p}}, \quad \frac{d\boldsymbol{p}}{dt} = -\frac{\partial H}{\partial \boldsymbol{r}} \qquad (3)$$

lead to the classical equation of motion

$$m\frac{d\mathbf{v}}{dt} = e(\boldsymbol{E} + \mathbf{v} \times \boldsymbol{B}) + \boldsymbol{F}_{non-em} \qquad (4)$$

where $\boldsymbol{F}_{non-em}(\boldsymbol{r}t) \equiv -\boldsymbol{\nabla}\mathrm{V}_{non-em}(\boldsymbol{r}t)$. The non-electromagnetic terms, if any, can be trivially added to the following argument, so for brevity I set $\boldsymbol{F}_{non-em} = \mathbf{V}_{non-em} = 0$.

The first Hamiltonian equation, $\frac{d\boldsymbol{r}}{dt} = \frac{\partial E}{\partial \boldsymbol{p}}$, simply yields the identity

$$\mathbf{v}(rt) \equiv \frac{dr(t)}{dt} = \frac{1}{m}(\boldsymbol{p} - e\boldsymbol{A}(rt)) \qquad (5)$$

The second Hamiltonian equation needs a little more care: using (4), we derive from it the equation

$$m\frac{d\mathbf{v}}{dt} = -\frac{\partial H}{\partial \boldsymbol{r}} - \frac{d\boldsymbol{A}(\boldsymbol{r}t)}{dt} \qquad (6)$$

Here it is important to note that the partial derivative $\partial H/\partial \boldsymbol{r}$ is taken at constant ρ and t, while the total derivative $\partial \boldsymbol{A}/dt$ is the sum of the partial derivative $\partial \boldsymbol{A}(\boldsymbol{rt})/\partial t$ at constant **r** and a "drift" term which written out explicitly in terms of the Cartesian components x_i of $\boldsymbol{r}$ and A_i of $\boldsymbol{A}$ is

$$\left.\frac{dA_i}{dt}\right|_{drift} = \sum_i \frac{dx_j}{dt}\frac{\partial A_i}{\partial x_j} \tag{7}$$

Similarly, written in terms of Cartesian components with summation over repeated indices assumed) we have

$$\frac{\partial H}{\partial x_i} = e\frac{\partial \Phi}{\partial x_i} + \mathrm{v}_j \frac{\partial}{\partial x_j} A_i \tag{8}$$

Thus, (6) becomes (since $\mathbf{v}$ is not a function of $\boldsymbol{r}$)

$$m\frac{\partial \mathrm{v}_i}{\partial t} = \left(-e\frac{\partial \Phi}{\partial x_i} + \frac{\partial A(rt)}{\partial t}\right) + \left(\mathrm{v}_j\frac{\partial A_j}{\partial x_i} - v_j\frac{\partial A_i}{\partial x_j}\right) \tag{9}$$

But the first two terms on the RHS of equation (9) are by equation (2b) just the total electric field E_i , while a simple vector identity yields for the second pair

$$\mathrm{v}_j\left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j}\right) \equiv [\mathbf{v}x(\boldsymbol{\nabla}\times\boldsymbol{A})]_i \tag{10}$$

Hence we recover from equation (9) the desired classical equation of motion equation (4), Q E D).