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Coulomb fields generated by minimal coupling*

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Abstract. In the ground state of an electrically charged spinless quantum particle, interacting with only the longitudinal part of the quantized electromagnetic field, the exact Coulomb potential is generated dynamically by minimal coupling if the non-electromagnetic mass of the particle vanishes and if the coupling constant (corresponding to renormalized charge) is such that $\alpha < \alpha_{crit} \approx 2.5$. Thus, contrary to classical expectations, Gauss' law need not be imposed as a physicality constraint in this case. For macroscopic values of the electric charge, the Coulomb field is energetically disfavoured. If the charged particle is assumed massive and non-relativistic, the ground state has an unphysical static background charge to which the particle is bound. In this case translational as well as gauge invariance is spontaneously broken.

1. Introduction

The breaking of a local chiral gauge symmetry by the ground state of the Higgs field is part of the standard scenario for the electroweak interaction. In ordinary gauge theories, on the other hand, local gauge invariance of states is conventionally enforced by imposing Gauss' law as a physicality constraint. The different treatment of ordinary and chiral gauge symmetries has recently been related to the non-existence of a chirally invariant lattice regularization [1]. In fact, for ordinary lattice QCD it had been shown heuristically [2] that even if the Gauss constraint is released the ground state would not break local SU(3) invariance. Thus the vacuum states in both kinds of gauge theory can be treated on the same formal basis. To what extent can Gauss' law be expected to hold automatically also for the ground states of the charged sectors in an ordinary gauge theory?

For 2+1-dimensional continuum Yang-Mills theory, the non-degeneracy of the unconstrained vacuum state in the temporal gauge was already derived in [3] by exploiting an analogy between the Yang-Mills Hamiltonian and non-relativistic ∞ -dimensional quantum mechanics. The argument of [2] is based on Wilson fermions and holds to all orders in the hopping-parameter and strong-coupling expansions. In fact, successive orders in these expansions are generated by gauge invariant operators B^2/g^2 in the strong coupling and $\kappa \bar{\psi} \gamma_0 \alpha \cdot (\nabla - iA) \psi$ in the hopping parameter series—while at zeroth order the Hamiltonian $g^2 E^2 + m \bar{\psi} \gamma_0 \psi$ has the gauge invariant ground state

$$\prod_{\text{links}} |E_l = 0\rangle \otimes \prod_{\text{sites}} |n_s = 0\rangle.$$

It is not in contradiction with classical expectations that the absolute ground state of

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an unconstrained local gauge theory would respect Gauss' law automatically. In the case of electromagnetism,

$$\nabla \cdot \mathbf{E}(\mathbf{x}) = \rho(\mathbf{x})$$

is clearly satisfied for the trivial solution of zero field strengths and charge densities. But in the presence of a charged particle, neglect of the Gauss constraint would still annul all Coulomb fields in the classical theory, thus leading to unphysical dynamical behaviour. In the classical ground state configuration the momentum of the particle as well as the unconstrained electric and magnetic field strength would exactly vanish. In quantum theory, however, such a configuration is in contradiction with the canonical commutation relations. As will be shown in the present paper, the quantum Gauss constraint is indeed redundant in this case for a certain range of dynamical parameters.

Not much seems to be known about the ground state of the Maxwell field with minimal coupling to a quantum particle. The related polaron problem of a quantum particle interacting with a scalar field has only been approximately solved using sophisticated variational techniques [4]. In order to enable a qualitative analysis, the transversal modes of the Maxwell field shall be neglected in the present paper. This should be a physically sensible simplification since Abelian local gauge invariance and the Coulomb fields accomplishing it are entirely contained in the longitudinal modes.

For a massive non-relativistic Schrödinger particle (section 2) the interacting ground-state properties can then be inferred from standard qualitative methods of quantum mechanics. The energetically favourable states have a non-dynamical background charge density (which is a measure of deviation from physicality) to which the particle is bound. The spatial extent of the bound state, as usual, is of the order of $1/\alpha$ Compton wavelengths. The background charge is an extended distribution, though; it exactly counters the *probability* density (not the intrinsic charge density) of the Schrödinger particle. This implies that the dynamically generated field of the particle vanishes on length scales greater than the Bohr radius but takes the Coulomb form, indeed, on length scales between the Bohr radius and the ultraviolet cut-off (the classical electron radius).

For a relativistic particle with zero non-electrostatic mass (section 3) the square-root kinetic energy requires the use of integral inequalities. (Due to the negative energy states the Dirac form of a relativistic kinetic energy is not appropriate for studying one-particle ground states.) In this case the qualitative ground state properties very much depend on the particle's electric charge. If $e^2/4\pi < 2.5$ the system behaves as expected by extrapolation from the non-relativistic case. The background charge distribution of total charge $-e$ then spreads out uniformly in space and is thus effectively absent. Consequently, the exact Coulomb field is generated by the dynamical mechanism inherent in the minimal coupling term of the Hamiltonian. If e^2 takes macroscopic values, however, the collapse of the Coulomb field becomes energetically favourable.

The relation of the semi-phenomenological model parameters m and e to the parameters of full QED is discussed in section 4.

2. Non-relativistic particle

A locally gauge invariant model of the charge-one sector of QED that can be qualitatively solved by standard methods of quantum theory is a charged non-relativistic quantum

particle interacting with only the longitudinal (Coulomb) modes of the quantized electromagnetic field. As for the choice of a quantization procedure, we shall start out from the temporal gauge in which the vector potential, even in the general non-Abelian case, is a Cartesian coordinate [5]. The canonically conjugate momentum is the electric field strength, and the canonical commutation relations can be postulated consistently in the standard form

$$[\hat{E}_k(x), \hat{A}_l(y)] = i\delta_{kl}\delta(x-y) \quad [\hat{E}_k(x), \hat{E}_l(y)] = 0 = [\hat{A}_k(x), \hat{A}_l(y)].$$

For the quantum particle the commutation relations are

$$[\hat{Q}_k, \hat{P}_l] = i\delta_{kl} \quad [\hat{Q}_k, \hat{Q}_l] = 0 = [\hat{P}_k, \hat{P}_l].$$

The complete temporal-gauge Hamiltonian of the minimally coupled system would be

$$H_{\text{exact}} = \frac{1}{2} \int (\mathbf{E}(x)^2 + (\nabla \times \mathbf{A}(x))^2) d^3x + \frac{1}{2m} (\hat{\mathbf{P}} - e\hat{\mathbf{A}}_{\text{reg}}(\hat{\mathbf{Q}}))^2 \quad (1)$$

where the 'reg' subscript denotes a smoothed-out particle-field interaction UV regularization with a charge distribution ρ_0 is defined for any function f by

$$f_{\text{reg}}(x) = \int f(x-y)\rho_0(y) d^3y. \quad (2)$$

The kinetic energy of a Schrödinger particle interacting with only the Coulomb modes of the gauge field is

$$H_{\text{kin}} = \frac{1}{2m} (\hat{\mathbf{P}} - e\hat{\mathbf{A}}_{\text{long reg}}(\hat{\mathbf{Q}}))^2. \quad (3)$$

The transversal modes, coupled in (1) to the longitudinal ones through the particle energy, are now dynamically independent and can be omitted from the following considerations. Thus the model Hamiltonian reads

$$H = \frac{1}{2} \int \hat{\mathbf{E}}_{\text{long}}(x)^2 d^3x + \frac{1}{2m} (\hat{\mathbf{P}} - e\hat{\mathbf{A}}_{\text{long reg}}(\hat{\mathbf{Q}}))^2.$$

Vacuum fluctuations are still present due to the non-commutativity of $\hat{\mathbf{E}}_{\text{long}}$ and $\hat{\mathbf{A}}_{\text{long}}$. They can be absorbed in the decoupling transformation

$$U_{\text{dec}} = \exp \left[ie \int \frac{\nabla \cdot \hat{\mathbf{A}}_{\text{reg}}(x)}{4\pi|x-\hat{\mathbf{Q}}|} d^3x \right]. \quad (4)$$

The effect of this transformation on the particle momentum $\hat{\mathbf{P}}$ can be obtained by using the commutator expansion $e^A B e^{-A} = B + [A, B] + \dots$ which here terminates at the first commutator:

$$\hat{\mathbf{P}}U_{\text{dec}} = U_{\text{dec}} \left(\hat{\mathbf{P}} + e\nabla_O \int \frac{\nabla \cdot \hat{\mathbf{A}}_{\text{reg}}(x)}{4\pi|x-\hat{\mathbf{Q}}|} d^3x \right).$$

The term added to $\hat{\mathbf{P}}$ just cancels the longitudinal vector potential in the kinetic energy. Likewise, the transformation adds a Coulomb field to the electric field strength operator,

$$\hat{\mathbf{E}}(x)U_{\text{dec}} = U_{\text{dec}} (\hat{\mathbf{E}}(x) + e\nabla_x (4\pi|x-\hat{\mathbf{Q}}|_{\text{reg}})^{-1}). \quad (5)$$

The Coulomb field is dependent on the particle position operator and is rendered finite by the regularization of the charge density.

We can now pull out the unitary factor U_{dec} of (4) from all states in the Hilbert space and transform the Hamiltonian accordingly

$$H' = U_{dec}^\dagger H U_{dec} = \frac{1}{2} \int (\hat{E}_{long}(x) + e \nabla_\nu (4\pi |x - \hat{Q}|_{reg}^{-1})^2 d^3x + \frac{\hat{P}^2}{2m}). \tag{6}$$

In this representation the longitudinal part of the vector potential is manifestly a cyclic variable only the conjugate momentum E_{long} occurs in H' , and it commutes with any other operator in the transformed Hamiltonian. Hence, by working in an E_{long} eigenbase, the eigenvalues ('eigenfields') of E_{long} can be treated as static background fields. As usual, we shall write the longitudinal E field and its eigenvalues as a gradient

$$\hat{E}_{long}(x) = \nabla \hat{\Phi}_{unph}(x) \tag{7}$$

The Φ field will later turn out to measure the deviations from Gauss' law. Inserting (7) into (6) we obtain the familiar form of the total energy for a particle in an electrostatic potential (E_{self} is the Coulomb self-energy)

$$H' = E_{self} + \frac{1}{2} \int (\nabla \Phi_{unph}(x))^2 d^3x + e \Phi_{unph reg}(\hat{Q}) + \frac{\hat{P}^2}{2m}$$

The carets have been dropped from the Φ s because we are now working in the Φ eigenbase. To determine the ground state of this Hamiltonian we first note that in a Φ eigenstate the only degrees of freedom left are those of the wavefunction of the Schrödinger particle, $\psi(q)$. Since only the eigenvalues of the Φ eigenstates enter the energy, the functionally continuum normalization of the eigenstates needs not be elaborated on here. It remains to determine the eigenfield $\Phi(x)$ and the one-particle wavefunction $\psi(q)$ such that the energy expectation value

$$\langle H' \rangle = E_{self} + \frac{1}{2} \int (\nabla \Phi_{unph}(x))^2 d^3x + \int \bar{\psi}(q) \left(-\frac{\Delta}{2m} + e \Phi_{unph reg} \right) \psi(q) d^3q$$

is an absolute minimum. This leads to the differential equations†

$$\Delta_x \Phi_{unph}(x) = e |\psi(x)|_{reg}^2 \tag{8}$$

$$\left(-\frac{\Delta_q}{2m} + e \Phi_{unph reg}(q) \right) \psi(q) = E \psi(q) \tag{9}$$

We obtain parameter-independent equations by the following substitutions:

$$\Phi_{unph}(x) \rightarrow me^3 \Phi_{unph}(me^2x) \quad \psi(q) \rightarrow (me^2)^{3/2} \psi(me^2q) \quad E \rightarrow me^4 E. \tag{10}$$

Equation (8) implies that Φ_{unph} behaves like $1/r$ at large distances. This guarantees that the ground state solution of (9) is a bound state with an exponential fall-off at large radii. The length scale of the fall-off is the inverse of me^2 as can be seen from (10).

We now discuss the physicality of the ground state

$$|0\rangle = U_{dec}(|\Phi_{unph}\rangle \otimes |\psi_0\rangle) \tag{11}$$

By the Ehrenfest theorem the expected value of $\nabla \cdot \hat{E}(x)$ should be zero everywhere which it is indeed. To see this we note that by (5) and (7)

$$\nabla \cdot \hat{E}(x) U_{dec} = U_{dec} (\Delta \hat{\Phi}_{unph}(x) - e \rho_0(x - \hat{Q})). \tag{12}$$

† There is a Lagrange multiplier (energy eigenvalue) only for the particle wavefunction, the variation of the eigenfield Φ is not restricted.

The expectation value of the first term on the RHS, taken with the ground state (11), is just $\Delta\Phi_{\text{unph}}(\mathbf{x})\langle\psi_0|\psi_0\rangle$ which is $e|\psi(\mathbf{x})|_{\text{reg}}^2$ by (8). The second term on the RHS of (12) gives $\langle\Phi_{\text{unph}}|\Phi_{\text{unph}}\rangle\int(-e)\rho_0(\mathbf{x}-\mathbf{q})|\psi_0(\mathbf{q})|^2d^3x$ and because of (2) this just cancels the previous term.

However, going beyond expectation values by decomposing the particle wavefunction ψ_0 into position eigenstates, we see from the RHS of (12) that there are two charge densities involved. (i) a background charge density $\Delta\Phi_{\text{unph}}$ which is independent of the particle position and which by (8) has the spatial extent of the particle wavefunction ψ_0 , and (ii) the particle's intrinsic charge density which is centred at the particle position and which has the spatial extent of the regulating function ρ_0 .

In the spatial domain to which the quantum particle is bound by the background charge the background electrostatic potential is thus not very strong in comparison with the particle's potential. In particular, the interaction with another charged particle (a test particle) would be dominated by the physical Coulomb potential in a region whose spatial extent is of the order of $1/(me^2)$ by (10).

In order to see whether the unphysicalities can be absent altogether, we now consider the limit $me^2 \rightarrow 0$. The limit of a massless Schrödinger particle, clearly, cannot be handled by the non-relativistic kinetic energy term (3).

3. Massless particle

In this section we replace the non-relativistic kinetic energy (3) with the massless relativistic analogue,

$$H_{\text{kin}} = ((\hat{\mathbf{P}} - e\hat{\mathbf{A}}_{\text{long reg}}(\hat{\mathbf{Q}}))^2)^{1/2}.$$

The first step of the analysis can be carried out unchanged. Pulling out the same unitary factor U_{dec} from all states in the Hilbert space and using the eigenbases of $\hat{\Phi}_{\text{unph}}$ and particle position again, we arrive at the following energy expectation value

$$\langle H' \rangle = E_{\text{self}} + \frac{1}{2} \int (\nabla\Phi_{\text{unph}}(\mathbf{x}))^2 d^3x + \int \bar{\psi}(\mathbf{q})(\sqrt{-\Delta_q} + e\Phi_{\text{unph reg}}(\mathbf{q}))\psi(\mathbf{q}) d^3q. \quad (13)$$

The action of $\sqrt{-\Delta}$ (a non-local operator) is defined as multiplication by $|\mathbf{p}|$ in the particle momentum space. The minimum of the total energy is now determined by the integro-differential equations

$$\Delta_x\Phi_{\text{unph}}(\mathbf{x}) = e|\psi(\mathbf{x})|_{\text{reg}}^2 \quad (14)$$

$$(\sqrt{-\Delta_q} + e\Phi_{\text{unph reg}}(\mathbf{q}))\psi(\mathbf{q}) = E_{\text{part}}\psi(\mathbf{q}). \quad (15)$$

As E_{self} is independent of the particle wavefunction and Φ_{unph} takes negative values by (14),

$$\min_{\psi, \Phi} \langle H' \rangle = E_{\text{self}} + E_{\text{part}} + \frac{1}{2} \int (\nabla\Phi_{\text{unph}}(\mathbf{x}))^2 d^3x = E_{\text{self}} + \langle (\mathbf{P}^2)^{1/2} \rangle + \frac{1}{2} \langle e\Phi_{\text{unph}}(\mathbf{Q}) \rangle.$$

It will be shown in the appendix that if the bare charge e is not too large, the minimum of the total energy is attained if the wavefunction of the relativistic Schrödinger particle spreads out over all space—the particle is not bound to a local fluctuation of the background charge. In fact,

$$\langle \psi | (\mathbf{P}^2)^{1/2} | \psi \rangle + \frac{1}{2} \langle \psi | e\Phi_{\text{unph}}(\mathbf{Q}) | \psi \rangle \geq (1 - Ce^2) \langle \psi | (\mathbf{P}^2)^{1/2} | \psi \rangle \quad (16)$$

where $C > 0$ is some constant depending on the quality of the estimates used. Thus, if $e^2 < C^{-1}$ the absolute minimum of the energy is attained (cf (13)) if: (i) the wavefunction approaches zero momentum (minimum of particle's total energy), and (ii) Φ_{unph} approaches a constant (minimum of unphysical electrostatic energy)

The maximal electric charge for which the estimate makes sense and for which physicality is an automatic property of the relativistic Schrödinger-particle ground state is

$$e_{\text{crit}}^2 = \frac{1}{C} = \inf_{\psi} \frac{\langle \psi | (\mathbf{P}^2)^{1/2} | \psi \rangle \langle \psi | \psi \rangle}{-\frac{1}{2} \langle \psi | \Phi_{\text{unph}}(\mathbf{Q}) | \psi \rangle} = \inf_{\psi} \frac{E_{\text{kin}}}{|E_{\text{Coul}}|} \quad (17)$$

where $\Phi_{\text{unph}}(\mathbf{x})$ solves the Poisson equation (14) and is itself proportional to $\langle \psi | \psi \rangle$. So far this author has been unsuccessful in solving the nonlinear optimization problem (17) by numerical methods. However, insertion of various analytically simple functions is suggestive of the numerical range in which the critical charge will lie. A selection of spherically symmetric wavefunctions is evaluated in table 1. It should be noted that the energy ratio to be minimized is scale invariant so that each of the wavefunctions represents a one-parameter family. As apparent from table 1,

$$\alpha_{\text{crit}} = \frac{e_{\text{crit}}^2}{4\pi} \approx 2.5.$$

By the correspondence principle, the quantum-dynamically generated Coulomb field is expected to break down for macroscopic values of the electric charge since without the Gauss constraint there would be no longitudinal electric fields in the lowest-energy state of a classical charged particle. In the present framework this breakdown shows up in that a spatially narrow wavefunction with an energy $\propto e^{2/3}/r_0$ is more favourable at large e^2 than a spread-out wavefunction with the Coulomb energy $\propto e^2/r_0$. In fact, for a given particle wavefunction the kinetic energy E_{kin} is independent of e^2 while E_{Coul} , the part of the field energy which depends on the wavefunction through (14), is proportional to $-e^2$. Once $E_{\text{kin}} + E_{\text{Coul}}$ takes a negative value it can be lowered further by conformal contraction of the wavefunction down to radii of the order of the regularization radius r_0 . The particle is then located in space and by (14) the unphysical longitudinal field no longer vanishes.

An upper bound on the total energy in this unphysical case can be obtained as follows. After the decoupling transformation U_{dec} it is sufficient for this estimate to consider an eigenstate of the longitudinal electric field with the eigenfield

$$\Phi_{\text{trial}}(\mathbf{x}) = \left[\frac{e}{4\pi|\mathbf{x} - \mathbf{q}_0|} \right]_{\text{reg}}.$$

Table 1. Some kinetic-to-Coulomb energy ratios

$n\psi(r)$	$E_{\text{kin}}/E_{\text{Coul}}$
$\exp(-r)$	∞
$r \exp(-r)$	34.1
$r^2 \exp(-r)$	35.2
$r \exp(-r^2)$	35.6
$\sin r, 0 \leq r \leq \pi$	100.0
$r/(1+r^2)$	39.4

This is not an exact solution of (14) and therefore not a local minimum of the energy expectation. Anticipating a spatially narrow particle wavefunction in the neighbourhood of q_0 we may expand, with respect to the particle displacement, the total field energy including the Coulomb self-energy analogous to the nonrelativistic equation (6):

$$\begin{aligned} E_{\text{field}} &= \frac{1}{2} \int \left(\nabla \Phi_{\text{trial}}(x) - \nabla \left[\frac{e}{4\pi|x-q|} \right]_{\text{reg}} \right)^2 d^3x \\ &= \sum_k (q - q_0)_i (q - q_0)_k \nabla_i \nabla_k \left[\frac{e^2}{4\pi|x|} \right]_{\text{reg}} \Big|_{x=0} = \frac{1}{3} e^2 (q - q_0)^2 \rho_0(0). \end{aligned}$$

Changing to momentum space and assuming $\rho_0(0) = 3/4\pi r_0^3$ as for a homogeneous charge distribution of radius r_0 , the total energy is given by the expectation value of the operator

$$|p| - \frac{e^2}{4\pi} \rho_0(0) \Delta_p.$$

The optimal particle wavefunction is an Airy function and the lowest eigenvalue of the total energy is [6]

$$2.3 \times \left[\frac{e^2}{4\pi} \right]^{1/3} \frac{1}{r_0}$$

4. Discussion

We have shown that the exact Coulomb field of a charged quantum particle is generated by minimal coupling to the longitudinal modes of the electromagnetic field, provided that the rest energy of the particle is entirely electrostatic and that the electric charge e is not larger than $e_{\text{crit}} \approx 6$. It remains to see if these requirements are consistent with full quantum electrodynamics. In fact, the bare charge of the electron, in the QED sense of the term, is infinite, but the total charge visible outside the domain of fermionic vacuum polarization around the electron position is such that $e^2/4\pi = \frac{1}{137}$ which would be small enough indeed for automatic generation of the Coulomb field. In the model considered here, only modes of the electromagnetic field with wavelengths larger than the radius of the smoothed-out charge distribution ρ_0 are coupled to the electron's charge distribution; it is thus the renormalized value of e which determines the effective strength of minimal coupling.

A mechanism that generates long-range fields for small coupling which collapse for $\alpha > 2.5$ is reminiscent of colour confinement. The corresponding scenario would be that Coulomb-like fields prevail at length scales in the asymptotically free regime, and that for more extended objects, in which the total colour charge has piled up to a critical value, a breakdown occurs by which the colour charge is rendered invisible outside.

The interpretation, in QED terms, of the bare mass parameter m as employed in the model may be approached by a comparison of self-energies. The classical electron radius r_0 is defined such that the electron mass coincides with the self-energy of the Coulomb field outside r_0 [7]; if m were to be identified with the remainder of the total electron rest energy it would be perfectly sensible to put it equal to zero. However, m might as well be identified by a comparison of self-momenta and will then, as usual

with classical models of the electron's internal structure [7], be different by a considerable factor depending on the details of the geometry assumed. The discrepancy between the masses derived from self-energy and self-momentum is particularly pronounced if the transverse modes of the electromagnetic field are decoupled from the particle: the electromagnetic part of the self-momentum then, in fact, vanishes.

To resolve the discrepancy in the interpretation of the mass parameter would require to include in some way the transverse modes of the vector potential in the energy estimates. Quantitatively, a comparison of energy expectations can be made for two distinguished states of the particle in interaction with the full electromagnetic field: for the product of a free particle wavefunction with the free electromagnetic vacuum, and for the analogous state in which the particle is dressed with its proper Coulomb field (an eigenstate of the electric field operator) at each particle position. Independently of whether the transverse modes are included or neglected in such a calculation, the Coulomb field is found to reduce the total energy [8].

Qualitatively, coupling the particle to the transverse modes would enhance its quantum fluctuations in configuration space so that the static components in the charge distribution operator would become less important. It is only for the static components, however, that Gauss' law requires more than its time derivative, which is essentially the (Hamiltonian) equation of continuity. Thus dynamical generation of Coulomb fields can be expected to occur as well for a quantum particle minimally coupled to the complete electromagnetic field.

Appendix. Estimating the unphysical Coulomb energy

We here prove the crucial inequality (16) for the automatic (unconstrained) gauge invariance of the relativistic one-particle ground state. The following standard definitions and integral inequalities will be used (notation of [9]): The p -norm of a function f in n dimensional space is defined by

$$\|f\|_p = \left[\int |f(x)|^p d^n x \right]^{1/p}.$$

For products of functions we have Hölder's inequality:

$$\|f \cdot g\|_r \leq \|f\|_p \|g\|_q \quad \text{for } 1/p + 1/q = 1/r.$$

For convolutions we have Young's inequality: let $f * g$ denote the convolution $\int f(x-y)g(y) d^n y$; then

$$\|f * g\|_r \leq \|f\|_p \|g\|_q \quad \text{where } 1/p + 1/q = 1 + 1/r.$$

A more specific case is Sobolev's inequality:

$$\iint \frac{|f(x)||h(y)|}{|x-y|^\lambda} d^n x d^n y \leq C_s \|f\|_p \|h\|_r \quad (18)$$

where in general $1/p + 1/r + \lambda/n = 2$ and $1 < p, r < \infty$ and the constant C_s depends on p, r, λ and n .

Fourier transforms can be estimated by the Hausdorff-Young inequality: let \tilde{f} denote the Fourier transform of f and let $1/p + 1/q = 1$ with $1 \leq q \leq 2$, then

$$\|f\|_p \leq C_{n,p} \|\tilde{f}\|_q.$$

Inequality (16) can now be derived as follows. By solving the Laplace equation (14) for Φ_{unph} we obtain the potential energy expectation of the Schrödinger particle

$$-\frac{1}{e^2} \langle \psi | e \Phi_{\text{unph}}(\mathbf{Q}) | \psi \rangle = \iint \frac{|\psi(\mathbf{x})|_{\text{reg}}^2 |\psi(\mathbf{y})|_{\text{reg}}^2}{4\pi|\mathbf{x}-\mathbf{y}|} d^3x d^3y.$$

To this expression we apply Sobolev's inequality; the case of interest here is $p = r = 6/5$, $n = 3$, $\lambda = 1$ and $f = g = |\psi|^2$. By Young's inequality and by the definition of regularization in (2),

$$\| |\psi|_{\text{reg}}^2 \|_p = \| |\psi|^2 \|_p \quad \text{for any } p$$

so the 'reg' subscript can be omitted here. By construction of the p -norm,

$$\| |\psi|^2 \|_p \equiv (\| \psi \|_{2p})^2 \quad (19)$$

so what we need is the 12/5-norm of the real-space Schrödinger wavefunction. It is related through the Hausdorff-Young inequality to the 12/7-norm of the wavefunction in momentum space,

$$\| \psi \|_{12/5} \leq C_{\text{HY}} \| \tilde{\psi} \|_{12/7} \quad (20)$$

Information about $\| \tilde{\psi} \|_{12/7}$ is provided by the normalization integral

$$1 = \int |\tilde{\psi}(p)|^2 d^3p = (\| \tilde{\psi} \|_2)^2$$

and by the kinetic energy expectation of the wavefunction,

$$\langle (\mathbf{P}^2)^{1/2} \rangle = \int |p| |\tilde{\psi}(p)|^2 d^3p = (\| p^{1/2} \tilde{\psi} \|_2)^2.$$

Exploiting the normalization by integrating over momenta $p < \mu$ only and using Hölder's inequality we obtain

$$\| \tilde{\psi} \|_{12/7} \leq \| 1 \|_{12} \| \tilde{\psi} \|_2 \leq (4\pi/3)^{1/12} \mu^{+1/4} \quad (p < \mu) \quad (21)$$

Exploiting the kinetic energy by integrating over momenta $p > \mu$ only and using Hölder's inequality again,

$$\begin{aligned} \| \tilde{\psi} \|_{12/7} &= \| p^{-1/2} (p^{1/2} \tilde{\psi}) \|_{12/7} \\ &\leq \| p^{-1/2} \|_{12} \| p^{1/2} \tilde{\psi} \|_2 \leq (4\pi/3)^{1/12} \mu^{-1/4} \| p^{1/2} \tilde{\psi} \|_2 \quad (p > \mu). \end{aligned} \quad (22)$$

In the total, by the triangle inequality for the 12/7-norm,

$$\| \tilde{\psi} \|_{12/7} \leq (\| \tilde{\psi} \|_{12/7})_{p < \mu} + (\| \tilde{\psi} \|_{12/7})_{p > \mu}.$$

Adding up (21) and (22) and optimizing [10] with respect to μ ,

$$\mu = (\| p^{1/2} \tilde{\psi} \|_2)^2 = \langle (\mathbf{P}^2)^{1/2} \rangle$$

we find

$$\| \tilde{\psi} \|_{12/7} \leq 2(4\pi/3)^{1/12} \langle (\mathbf{P}^2)^{1/2} \rangle^{1/4}.$$

Finally, returning through (20), (19) and (18) to the estimate (16) of the 'unphysical' Coulomb energy in terms of the particle's bare momentum, we see that the constant in the inequality is not greater than

$$C = 8(4\pi)^{1/3} C_S C_{\text{HY}}$$

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