Kivelson *et al.* Reply: The extended Hubbard Hamiltonian includes only interactions between electron site-charge densities and hence ignores the explicit repulsion between bond-charge densities. Our Letter addressed the missing bond charge and the physical consequences of correctly adding the bond charge to the model.

We considered the effect of electron-electron (e-e) interactions on the equilibrium lattice dimerization in one dimension (as might be appropriate to a conducting polymer such as polyacetylene). In the extended Hubbard model with a half-filled band and a fixed value of the electron-phonon interaction, the magnitude of the dimerization is an increasing function of the strength of the electron-electron interaction over a wide range of parameters.[1,2] Since the lattice dimerization produces a bond-charge–density wave, we argued[3] that this must be an artifact of the model since e-e repulsion should favor a state of uniform charge density. By including the bond-charge repulsion (W) as well as the on-site (U) and nearest-neighbor site (V) repulsions, we showed explicitly that so long as as $3W > V$, then to first order the electron-electron interactions tend to oppose dimerization.

The Comments[4] of Baeriswyl, Horsch, and Maki and of Gammel and Campbell question two aspects of our analysis: (1) They both argue that for a realistic model of the electron-electron interactions, $V \gg W$ and hence W can be ignored. (2) Gammel and Campbell argue that in addition, since $U \gg V$ and W, and since in second order U tends to increase dimerization, even in the case where $W \sim V$, interactions tend to increase dimerization.

We consider these in turn. Let $\phi_n(r)$ be the Wannier function associated with the site n. Then

$$W = \int d^3r_1 d^3r_2 \phi_n^*(\mathbf{r}_1)\phi_{n+1}(\mathbf{r}_1) \times v(\mathbf{r}_1 - \mathbf{r}_2)\phi_{n+1}^*(\mathbf{r}_2)\phi_n(\mathbf{r}_2), \quad (1)$$

where $v(\mathbf{r})$ is the electron-electron interaction, and

$$V = \int d^3r_1 d^3r_2 |\phi_n(\mathbf{r}_1)|^2 v(\mathbf{r}_1 - \mathbf{r}_2) |\phi_{n+1}(\mathbf{r}_2)|^2. \quad (2)$$

For $v(\mathbf{r}) = \delta(\mathbf{r})$, it is easy to show that $W = V$, whereas for infinite-range interactions, $W = 0$ because of the orthogonality of ϕ_n and ϕ_{n+1}. The fact that $W \ll V$ for an unscreened Coulomb interaction reflects the fact that $v(\mathbf{r})$ is slowly varying on the length scale over which $\phi_n(\mathbf{r})$ falls to zero.

The basic validity of the extended Hubbard model as applied to real systems rests on the assumption that the electron-electron interactions have been self-consistently screened and that the residual interactions that appear explicitly in the model are the screened interactions. Thus, we conclude that for a consistent and realistic model, it is a reasonable approximation[5] to take $v(\mathbf{r}) = (e^2/r)e^{-\kappa r}$, where κ^{-1} is an appropriate (e.g., Thomas-Fermi) screening length, $\kappa^{-1} \simeq 1$–2 Å for a system such as polyacetylene with $\approx 5 \times 10^{22}$ π electrons per unit volume. For given ϕ_n, it is straightforward to calculate W and V with this screened interaction.

To make the calculations analytically tractable, we approximate $v(\mathbf{r})$ by Gaussian screening, $v(\mathbf{r}) = (e^2/r) \times \exp[-(\kappa r)^2]$. We do not expect this to introduce serious error, since it preserves the important features that $v(r) \sim e^2/r$ for $\kappa r < 1$ and $v(r)$ goes rapidly to zero for $\kappa r > 1$. We also approximate the Wannier functions in terms of Gaussians,

$$\tilde{\phi}_n(\mathbf{r}) = (2\lambda^2/\pi)^{3/4} \exp[-\lambda^2(\mathbf{r} - \mathbf{R}_n)^2],$$

where $\mathbf{R}_n$ is the position of the nth site. Since the $\tilde{\phi}_n$ are not orthogonal we orthogonalize them on different sites to obtain the actual Wannier functions ϕ_n. For simplicity, we consider the two-site problem where the orthogonalization is straightforward. In this case,

$$U = U_0[2 - S^2 + 2S^4 + S^2A - 4S^2B], \quad (3a)$$

$$V = U_0[S^2 + 2S^4 + (2 - S^2)A - 4S^2B], \quad (3b)$$

$$W = U_0 S^2[3 + A - 4B], \quad (3c)$$

where

$$U_0 = (2/\pi)^{1/2}(e^2/\lambda a^2)\beta^2/(1 - S^2)^2,$$

and $S = \exp[-1/2(\lambda a)^2]$ is the overlap function. The other quantities which enter into Eqs. (3a)–(3c) are as follows: $A = e^{-\alpha} f(\beta)$, $B = e^{-\alpha/4} f(\beta/2)$, $\alpha = \kappa^2 a^2 z^2$, $z^2 = \lambda^2/(\lambda^2 + 2\kappa^2)$, $\beta = \lambda a z/\sqrt{2}$, $f(x) = (\pi^{1/2}/x)\mathrm{erf}(x)$, where $\mathrm{erf}(x)$ is the error function, and a is the distance between the two sites. For example, at $\lambda = \kappa = a^{-1}$, $W/U \approx V/U \approx 0.7$. We conclude that, in keeping with our physical arguments, bond-charge repulsion (W) is typically as important as the nearest-neighbor repulsion (V) under conditions appropriate to real systems.

Of course, the on-site interaction, U, is typically larger than either V or W. While in first order U does not affect the equilibrium dimerization, in second order (i.e., to order $U^2/2\pi t_0$, where t_0 is the transfer integral) it leads to an enhanced dimerization.[1,2] This effect has been found in Monte Carlo calculations to persist out to $U \approx 4t_0$. However, except at very small values of the dimerization, the effect of U is never very large; for the value of the electron-phonon coupling constant originally used by Su, Schrieffer, and Heeger[6] in their study of polyacetylene, Monte Carlo calculations indicate that the dimerization is increased by a maximum of 20% for $U \approx 2t_0$. This is small compared to the first-order effect from W (and V) unless $|3W - V| \ll U$.

Our conclusion is consistent with the recent work of Wu, Sun, and Nasu,[7] who start from the full Coulomb interaction with any strength and range. They find that when the interaction range is of the order of a lattice constant, the bond alternation monotonically decreases with increasing interaction strength.

We conclude with a comment concerning the meaning of the term "realistic parameters" in any Hubbard-type model. It is, of course, obvious that the neglect of electron-electron interactions is never justified in a solid; however, in many cases, such as in normal metal, the physics *can most easily* be described in terms of weakly interacting quasiparticles. While there are some fundamental problems associated with defining a Fermi-liquid theory in a one-dimensional metal, quasiparticle description of a one-dimensional semiconductor, such a polyacetylene, is quite straightforward.[5] Thus, the electron-phonon coupling and the Hubbard-model interactions should always be viewed as Fermi-liquid parameters in which screening, and other high-energy effects, have already been taken into account.

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